BNL 21714

CRYSNET MANUAL

Informal Report

July 1976

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To: Users of CPRØGS programs

From: Frances C. Bernstein 6/7/76

7600: From now on, our standard 7600 program binaries will be maintained in the following places:

1. SN=CHEM ID=CPRØGS
2. SN=ISTRY ID=CPRØGS
3. main catalog (SN=SYSTEM default) will have only

```
ACCESS , ID=ZZGCPRØGS
CALCMP , ID=ZZGCPRØGS
SETCMA , ID=ZZGCPRØGS
RMCØPY , ID=ZZGCPRØGS
CPRØGS , ID=ZZGCPRØGS        directory
MAKBIN , ID=ZZCCPRØGS
MAKBCDS, ID=ZZGCPRØGS
MAKBCDL, ID=ZZGCPRØGS
WHATIS , ID=ZZGCPRØGS
```

4. Tape (7 track)

Thus there are two common ways to use the programs.

1. Attach the programs from a private pack or from the main catalog if it is known to be there.
2. Use ACCESS to find a binary and put it in the catalog. In this case it is important to know that <u>ACCESS will no longer be available with ID=CPRØGS</u>. Thus one must

   ATTACH(ACCESS,ID=ZZGCPRØGS)

   and then ACCESS(___,ID=CPRØGS).
   This will search for the binary in the following order

   1. ___,ID=CPRØGS
   2. ___,ID=ZZGCPRØGS
   3. ___,ID=CPRØGS, SN=CHEM (or ISTRY)
      if CHEM (or ISTRY) is mounted
   4. Tape

   When the binary is found it will be put in the main catalog (under ID=ZZGCPRØGS) with the account number of the job doing the ACCESS. The default retention period, in this case, is one day but a longer retention period may be defined on the ACCESS card by the RP parameter. Note that permanent file storage is very expensive.

   At present, if ACCESS has to use a tape to find the binary (i.e. if a pack is not mounted) it is able to use a tape even if the job has TPO on the job card.

6600: The following 6600 binaries will be maintained in the main catalog

```
ACCESS , ID=CPRØGS
CALCMP , ID=CPRØGS
SETCMA , ID=CPRØGS
RMCØPY , ID=CPRØGS
EDIT   , ID=CPRØGS
BUPD140, ID=CPRØGS
MAKBIN , ID=CPRØGS
MAKBCDS, ID=CPRØGS
MAKBCDL, ID=CPRØGS
CPRØGS , ID=CPRØGS          directory
```

As in the past any other binaries are obtained by

```
ATTACH(ACCESS,ID=CPRØGS)
ACCESS(___,ID=CPRØGS)
```

and it is necessary to specify MT1 on the job card if the tape will be used by ACCESS.

For further information please consult the ACCESS writeup or speak to F. Bernstein or H. Bernstein.

General Notes

1. Anyone who wishes to receive additions and corrections to his/her copy of the CRYSNET manual should complete the attached form and include 20 removable labels with address typed on. An attempt will then be made to keep all such manuals current.

2. Please notify Frances C. Bernstein, Thomas F. Koetzle or Herbert J. Bernstein of any errors or problems in the use of this manual or any programs described.

3. Most writeups which include control cards show

```
ATTACH(__,ID=LPRØGS)
```

to localize binary of the desired program. Because of heavy permanent file changes most programs can no longer be localized in that way. The following is a brief description of the new procedure for each machine.

7600: Using the disk pack one must put YD1 as one of the parameters on the job card, i.e.

```
JØB,CP70,YD1.
ACCØUNT(__,__)
MØUNT(VSN=CHEMO1,SN=CHEM)
ATTACH(__,ID=CPRØGS,SN=CHEM)
```

One may currently use TPO which indicates no tapes for such a job provided there are no other uses of magnetic tape. Mounts are usually performed very quickly but, if large charges are imposed for them, one may have to use ACCESS as follows

```
JØB,CP70.
ACCØUNT(__,__)
ATTACH(ACCESS,ID=CPRØGS)
ACCESS(__,ID=CPRØGS)
```

ACCESS will bring the program in from tape and CATALØG it if the binary is not already in the catalog. Because tape might be used one may not specify TPO on the job card unless one is certain that the binary has already been put in the catalog.

6600: One must use ACCESS to bring binary in from tape unless it is already in the catalog

```
JØB,MT1.
ACCØUNT(__,__)
ATTACH(ACCESS,ID=CPRØGS)
ACCESS(__,ID=CPRØGS)
```

The MT parameter specifies the maximum number of 7-track magnetic tapes in simultaneous use for the job and may need adjustment for a particular job.

4. DISPØSE is of great use in directing files to a given terminal and in segmenting these files. See enclosed memo.

5. The source code for all the programs is available on an ØLDPL using CDC UPDATE. The ØLDPL is available on magnetic tape C206 (record type S must be specified on the 7600). The ØLDPL is also on the 7600 disk pack as ØLDPL,ID=CPRØGS and is also record type S.

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I wish to receive updates to the CRYSNET manual. I have included 20 prepared mailing labels.

Name and address:

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I. INTRODUCTION

THIS MANUAL DESCRIBES THE HARDWARE AND SOFTWARE WHICH TOGETHER MAKE UP THE CRYSTALLOGRAPHIC COMPUTING NETWORK (CRYSNET). THE MANUAL IS INTENDED AS A USERS GUIDE AND ALSO PROVIDES GENERAL INFORMATION FOR PERSONS WITHOUT ANY EXPERIENCE WITH THE SYSTEM.

CRYSNET IS A NETWORK OF INTELLIGENT REMOTE GRAPHICS TERMINALS (FIGURE I-1) THAT ARE USED TO COMMUNICATE WITH THE CDC CYBER 70/76 COMPUTING SYSTEM AT THE BROOKHAVEN NATIONAL LABORATORY (BNL) CENTRAL SCIENTIFIC COMPUTING FACILITY (CSCF). TERMINALS ARE IN ACTIVE USE BY FOUR RESEARCH GROUPS IN THE FIELD OF CRYSTALLOGRAPHY, LOCATED AT BNL, THE INSTITUTE FOR CANCER RESEARCH (ICR), JOHNS HOPKINS UNIVERSITY, AND TEXAS A AND M UNIVERSITY. A FIFTH GROUP, AT THE MEDICAL FOUNDATION OF BUFFALO, HAS USED A TERMINAL WITHOUT GRAPHICS CAPABILITY TO COMMUNICATE WITH BNL ON A LESS FREQUENT BASIS THAN THE FOUR GROUPS MENTIONED ABOVE.

A PROTEIN DATA BANK HAS BEEN ESTABLISHED AT BNL, TO STORE IN MACHINE-READABLE FORM ATOMIC COORDINATES AND OTHER CRYSTALLOGRAPHIC DATA FOR MACROMOLECULES. THE DATA BANK OPERATES IN COLLABORATION WITH THE CRYSTALLOGRAPHIC DATA CENTRE (CAMBRIDGE, ENGLAND), AND DISTRIBUTES DATA UPON REQUEST TO MEMBERS OF THE SCIENTIFIC COMMUNITY. THE BANK CURRENTLY INCLUDES DATA FOR MORE THAN 20 PROTEINS. THIS STRUCTURAL INFORMATION CAN BE ACCESSED AT BNL DIRECTLY BY THE CRYSNET GRAPHICS TERMINALS.

MORE THAN TWO YEARS OF EXPERIENCE HAS BEEN ACCUMULATED WITH CRYSNET. DURING THIS PERIOD, IT HAS BEEN DEMONSTRATED THAT THE TERMINALS, WHICH PROVIDE ACCESS TO A LARGE, FAST THIRD-GENERATION COMPUTER, PLUS STAND-ALONE INTERACTIVE GRAPHICS CAPABILITY, ARE USEFUL FOR COMPUTATIONS IN CRYSTALLOGRAPHY, AND IN A VARIETY OF OTHER APPLICATIONS AS WELL. BATCH AND INTERACTIVE JOBS MAY BE RUN FROM THE TERMINALS ON THE CYBER 70/76. THE TERMINALS CAN ALSO BE USED TO COMMUNICATE WITH COMPUTING CENTERS OTHER THAN THAT AT BNL, ALTHOUGH IN THE CASE OF NON-CDC CENTERS THIS REQUIRES THE ACQUISITION OF APPROPRIATE ADDITIONAL COMMUNICATIONS SOFTWARE FOR THE TERMINALS. SMALL COMPUTATIONS ARE CONVENIENTLY CARRIED OUT ON THE TERMINAL MINICOMPUTERS THEMSELVES, AND A LIBRARY OF SUITABLE ROUTINES FOR CRYSTALLOGRAPHIC CALCULATIONS HAS BEEN ASSEMBLED.

INTERACTIVE GRAPHICS IS NATURALLY OF GREAT UTILITY FOR THE EXAMINATION OF MOLECULAR STRUCTURES. WITH THE SOFTWARE PRODUCED FOR THE CRYSNET TERMINALS (PDP 11/40-VECTOR GENERAL COMBINATION), IT IS POSSIBLE TO DISPLAY QUITE LARGE STRUCTURES WITH UP TO SEVERAL THOUSAND ATOMS, STARTING FROM A LIST OF ATOMIC COORDINATES. MODELS CAN BE VIEWED IN STEREO, MANIPULATED IN REAL TIME, AND ROTATED TO PRODUCE A REALISTIC KINETIC-DEPTH EFFECT. SOFTWARE HAS BEEN DEVELOPED TO DISPLAY MOLECULAR MODELS SUPERIMPOSED UPON CONTOURED ELECTRON-DENSITY MAPS, AND THIS "ELCTRONIC RICHARDS BOX" PROGRAM IS CURRENTLY BEING USED IN ATTEMPTS TO FIT A MODEL OF THE PROTEIN STAPHYLOCOCCAL NUCLEASE TO ITS HIGH-RESOLUTION ELECTRON-DENSITY MAP. THUS, IN ADDITION TO MANY DEMONSTRATED ADVANTAGES FOR THE DISPLAY OF STRUCTURAL RESULTS, THE CRYSNET GRAPHICS TERMINALS ARE PROVING TO BE USEFUL IN THE SOLUTION AND REFINEMENT OF STRUCTURES.

THE PRESENCE OF THE CRYSNET TERMINALS IN A CHEMISTRY DEPARTMENT, TWO BIOPHYSICS DEPARTMENTS, AND A CANCER RESEARCH CENTER, HAS LED IN THE RELATIVELY SHORT SPAN OF TWO AND A HALF YEARS TO THE EXPOSURE OF SCIENTISTS FROM A RANGE OF DISCIPLINES TO MINICOMPUTERS AND COMPUTER GRAPHICS. A NUMBER OF EXCITING NON-CRYSTALLOGRAPHIC APPLICATIONS OF GRAPHICS HAVE BEEN EXPLORED. THESE INCLUDE THE STUDY OF CHEMICAL-REACTION PATHWAYS, DISPLAY OF THEORETICAL ELECTRON-DENSITY MAPS, EXPLORATION OF MOLECULAR CONFORMATIONS DEDUCED FROM NMR DATA, AND A VARIETY OF PEDAGOGICAL USES.

THE IMPLEMENTATION OF CRYSNET HAS INVOLVED A LARGE COMMITMENT TO DEVELOP GRAPHICS SOFTWARE WRITTEN FOR A PARTICULAR TERMINAL HARDWARE CONFIGURATION. SINCE COMPUTER GRAPHICS HARDWARE IS EVOLVING RAPIDLY, IT HAS BEEN IMPORTANT TO MAKE THE SOFTWARE ADAPTABLE TO OTHER HARDWARE CONFIGURATIONS. THEREFORE, THE DECISION WAS MADE TO WRITE AS MUCH OF THE GRAPHICS SOFTWARE AS POSSIBLE IN A HIGHER-LEVEL LANGUAGE, NAMELY FORTRAN. THIS DECISION HAS PAYED OFF, AND THE BASIC MOLECULAR DISPLAY PACKAGE FOR THE PDP 11/VECTOR GENERAL SYSTEM HAS BEEN MODIFIED TO RUN INTERACTIVELY ON THE CDC 6600, AND TO DRAW PICTURES ON A TEKTRONIX STORAGE-TUBE TERMINAL AT JOHNS HOPKINS. SOME OF THE GRAPHICS ROUTINES HAVE ALSO BEEN MODIFIED TO RUN ON A NOVA COMPUTER.

IN THE SUCCEEDING SECTIONS OF THIS MANUAL, WE WILL DESCRIBE IN SOME DETAIL THE TERMINAL HARDWARE, THE ACTUAL OPERATIONS OF THE TERMINALS, OPERATIONS OF THE BNL CENTRAL FACILITY, AND GIVE DOCUMENTATION OF THE TERMINAL AND CENTRAL-SITE SOFTWARE.

CRYSNET IS ONE OF A NUMBER OF PIONEERING EFFORTS IN THE USE OF COMPUTER NETWORKING IN CHEMISTRY AND BIOCHEMISTRY, AND INVOLVES A COMPLEX COLLABORATIVE EFFORT AMONG SEVERAL INSTITUTIONS.
ACKNOWLEDGEMENT IS DUE FOR THE SPECIAL CONTRIBUTIONS TO CRYSNET OF LAWRENCE C. ANDREWS, HELEN M. BERMAN, FRANCES C. BERNSTEIN, HERBERT J. BERNSTEIN, GRAHAM H. CAMPBELL, H. L. CARRELL, H. B. CHIANG, WALTER C. HAMILTON, JONATHAN C. HANSON, DANIEL D. JONES, DAVID KLUNK, THOMAS F. KOETZLE, EDGAR F. MEYER, CARL N. MORIMOTO, SUSAN M. SEVIAN, R. KING STODOLA, MORRIS M. STRONGSON, STANLEY M. SWANSON, GRAHEME J. B. WILLIAMS, AND THOMAS V. WILLOUGHBY. IN ADDITION TO THESE INDIVIDUALS, MANY USERS OF THE SYSTEM HAVE, THROUGH THEIR COMMENTS AND ENTHUSIASM, HELPED CRYSNET TO GROW. THE EFFORTS OF ALL THESE USERS ARE DEEPLY APPRECIATED.

ANY COMMENTS OR CRITICISM SHOULD BE DIRECTED TO

CRYSNET PROJECT
BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT
BUILDING 555A
UPTON, L.I., NEW YORK 11973

OR TELEPHONE 516-345-4379/4384 ON THE BELL SYSTEM (664-4379/4384 ON FTS).

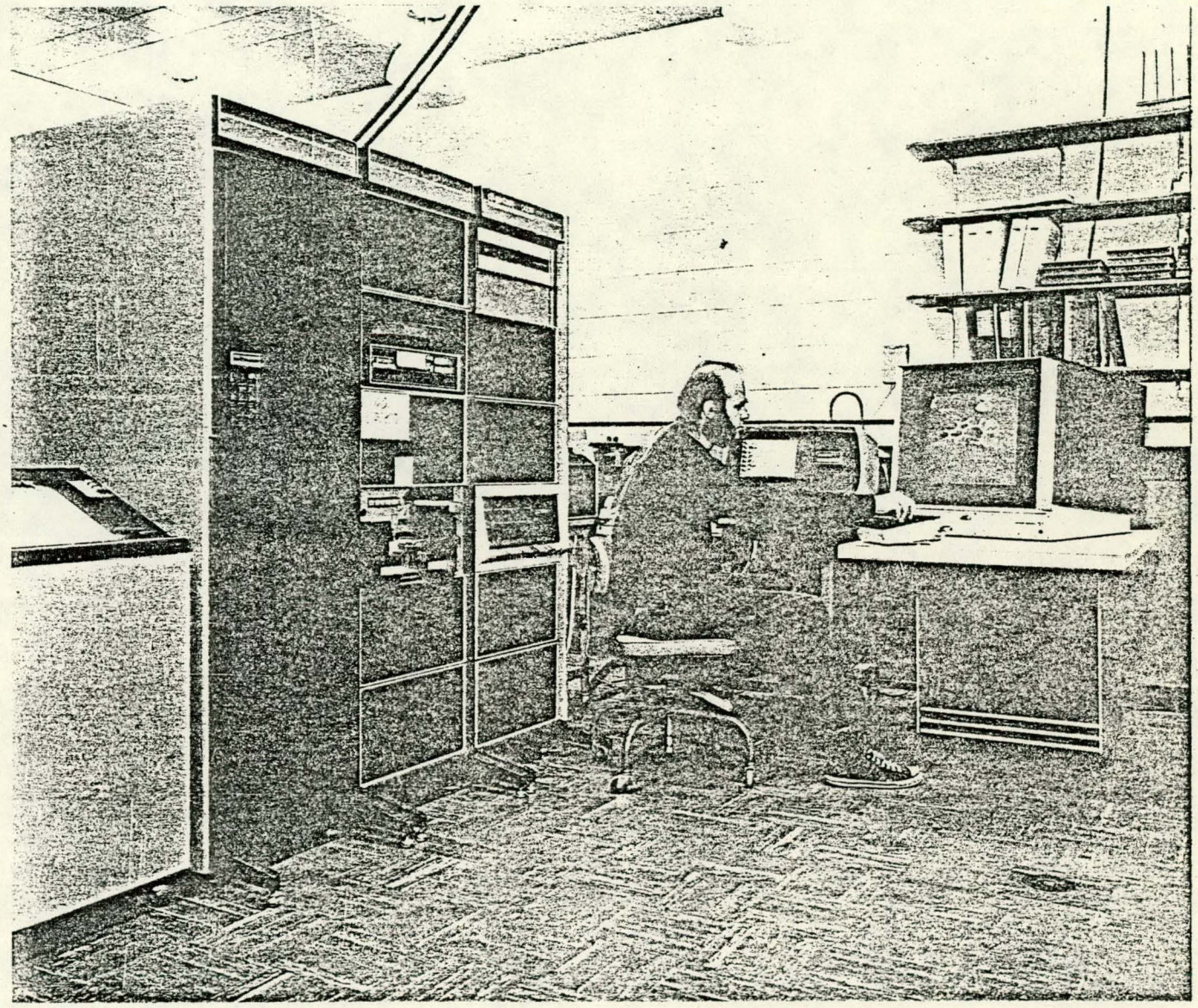

FIGURE I-1 - CRYSNET TERMINAL

II. CRYSNET TERMINAL HARDWARE AND SYSTEM SOFTWARE

THE HARDWARE CHOSEN FOR THE CRYSNET TERMINAL WAS SELECTED FROM COMMERCIALLY AVAILABLE COMPONENTS. THOUGH SOME OF THE ORIGINAL COMPONENTS OF THE TERMINAL ARE NO LONGER READILY AVAILABLE, THEY ALL HAVE CURRENT FUNCTIONAL EQUIVALENTS. IF ONE ASSEMBLES A TERMINAL FROM PRECISELY SUCH COMPONENTS, THEN THE EXISTING SOFTWARE WILL RUN WITHOUT ALTERATION. IF LOCAL REQUIREMENTS MANDATE CHANGES, THERE IS VERY LIKELY TO BE SOME IMPACT ON THE SOFTWARE, RANGING FROM TRIVIAL CONVERSIONS OF SUBROUTINES AND DEVICE DRIVERS, ALL THE WAY TO TOTAL RECREATION OF THE SOFTWARE PACKAGE. WE WILL ATTEMPT TO ASSESS THE IMPACT OF SOME LIKELY CHANGES. THIS SHOULD ALLOW THE READER TO EXTRAPOLATE TO THE PRECISE CHANGES ONE MIGHT CONTEMPLATE.

ALONG WITH THE HARDWARE, SOME COMMERCIALLY AVAILABLE SYSTEM SOFTWARE PACKAGES HAVE BEEN OBTAINED. THESE SERVE AS A BASE FOR THE REST OF THE SOFTWARE. SOME NECESSARY CHANGES HAVE BEEN MADE IN THESE PACKAGES, SO THERE WOULD BE A NON-TRIVIAL IMPACT WERE ONE TO SELECT EVEN DIFFERENT VERSIONS OF PRECISELY THE SAME PACKAGES. WE WILL ATTEMPT TO ASSESS THIS IMPACT AS WELL AS THAT FOR HARDWARE CHANGES.

I. OVERVIEW OF THE HARDWARE

THE MAJOR HARDWARE COMPONENTS OF THE TERMINAL ARE:

MINICOMPUTER WITH DISC AND MAGTAPE
DISPLAY SYSTEM
COMMUNICATIONS GEAR
PRINTER/PLOTTER
CARD READER

THE MINICOMPUTER SEES THE OTHER DEVICES AS PERIPHERALS, AND PROVIDES CENTRAL CONTROL OF THEIR OPERATION. THE COMMUNICATIONS GEAR PROVIDES AN INTERFACE BETWEEN THE COMPUTER AND A LINE TO THE CENTRAL COMPUTER. THE DISPLAY SYSTEM PROVIDES INTERACTIVE DISPLAY OF IMAGES STORED IN THE MINICOMPUTER. THE PRINTER/PLOTTER PROVIDES A PERMANENT RECORD OF THE DISPLAY SYSTEM IMAGES, AND PRINTED RECORDS OF PROGRAMS RUN EITHER ON THE MINICOMPUTER OR AT THE CENTRAL SITE. THE CARD READER PROVIDES A MEANS OF USER DATA INPUT TO THE SYSTEM. THE MAGTAPE ON THE MINICOMPUTER IS ALSO USED FOR DATA INPUT, ESPECIALLY FROM EXPERIMENTAL DEVICES AND OTHER COMPUTERS. SINCE THERE IS NO DIRECT CROSS-CONNECTION BETWEEN THE PERIPHERALS, IT IS POSSIBLE TO OMIT, SAY, THE COMMUNICATIONS GEAR AND STILL HAVE A VIABLE DISPLAY SYSTEM. ALTERNATIVELY, ONE MAY ADD OTHER COMPONENTS, SUCH AS PAPER TAPE EQUIPMENT, WITHOUT LOSS OF THE EXISTING FUNCTIONS. THUS THE HARDWARE CONSTITUTES A REASONABLY STANDARD INTELLIGENT REMOTE BATCH GRAPHICS TERMINAL.

THE MINICOMPUTER CHOSEN IS A DIGITAL EQUIMENT CORPORATION (DEC) PDP-11/40. THERE ARE MANY EQUIVALENT MACHINES AVAILABLE FROM OTHER VENDORS. ONCE ASSEMBLY LANGUAGE DEVICE DRIVERS FOR THE DISPLAY, COMMUNICATIONS GEAR, OPERATOR CONSOLE, AND PRINTER/PLOTTER HAVE BEEN CONVERTED, THE REST OF THE SOFTWARE SHOULD NOT PRESENT INSURMOUNTABLE

PROBLEMS, SINCE IT IS WRITTEN LARGELY IN FORTRAN. THE PRINCIPAL REQUIREMENT IS THAT ONE HAVE SOURCE OF ESSENTIAL SYSTEM PROGRAMS, OR ASSURANCE THAT THE DESIRED FEATURES ARE ALREADY PRESENT. THE SINGLE MOST DIFFICULT TASK WOULD BE THE CONVERSION OF THE COMMUNICATIONS CODE. THIS COULD EASILY ABSORB FOUR MAN-MONTHS OF A SKILLED PROGRAMMER. THE SECOND TASK WOULD BE TO PREPARE A SUPPORT PACKAGE FOR THE DISPLAY, WHICH COULD REQUIRE ALMOST AS MUCH TIME. FOR SOME OTHER MACHINES, SUCH AS THE DATA GENERAL NOVA, PACKAGES FOR THESE PURPOSES ALREADY EXIST, SHARPLY REDUCING THE REQUIRED EFFORT.

THE DISPLAY CHOSEN IS A VECTOR GENERAL 3D2. THIS DISPLAY PROVIDES REAL-TIME ROTATION OF DEPTH-CUED IMAGES OF VERY HIGH RESOLUTION. MUCH OF THE DISPLAY SOFTWARE, WHILE WRITTEN IN FORTRAN, DOES ASSUME AN ARCHITECTURE ALLOWING THE USE OF 3 BY 3 TRANSFORMS TO CONTROL THE PRESENTATION OF A PREVIOUSLY DRAWN DISPLAY. WITHOUT THIS FEATURE, REAL-TIME INTERACTION WOULD BE LOST, SINCE THE CPU CHOSEN IS NOT POWERFUL ENOUGH TO TOTALLY REDRAW IMAGES IN ONE FRAME TIME. THUS IT IS LIKELY THAT CONVERSION TO A POWERFUL SYSTEM SUCH AS EVANS AND SUTHERLAND'S PICTURE SYSTEM WOULD BE POSSIBLE WITHOUT LOSS OF FEATURES. CONVERSION TO LESS POWERFUL DISPLAYS, SUCH AS TECTRONIX STORAGE TUBES, WOULD ENTAIL A LOSS OF MOST REAL-TIME INTERACTION.

ADDITIONAL COMPONENTS WERE CHOSEN FROM THOSE AVAILABLE WHICH HAD INTERFACES TO THE PDP 11/40. IT SHOULD BE NOTED THAT THE EQUIPMENT WAS NOT OBTAINED FROM A SINGLE VENDOR. THIS RESULTED IN A LOWER PRICE FOR SOME COMPONENTS. IF ONE DOES NOT WISH TO FACE THE PROBLEMS OF DEALING WITH MULTIPLE VENDORS, IT IS POSSIBLE TO PURCHASE ALL OF THE TERMINAL THROUGH, SAY, THE DISPLAY VENDOR. MORE SERIOUS THAN PURCHASE PROBLEMS IN A MULTIPLE VENDOR SITUATION ARE MAINTENANCE PROBLEMS. UNLESS ONE HAS EXTREMELY GOOD IN-HOUSE MAINTENANCE, ONE MUST ARRANGE CONTRACTS FOR SERVICE WITH EITHER THE VENDORS OR A SERVICE ORGANIZATION. FOR THE COMPONENTS CHOSEN, SUCH CONTRACTS ARE AVAILABLE, AND DO SEEM TO PROVIDE ADEQUATE COVERAGE. IF SUBSTITUTIONS ARE MADE ONE MUST CAREFULLY VERIFY THE AVAILABILITY OF SERVICE.

IN ADDITION TO ARRANGING SERVICE FOR THE SYSTEM, ONE MUST ALSO INSURE ADEQUATE SUPPLIES, POWER, ENVIRONMENTAL CONTROL, AND IN-HOUSE SUPPORT.

2. OVERVIEW OF THE SYSTEM SOFTWARE

THE MAJOR SYSTEM SOFTWARE COMPONENTS OF THE TERMINAL ARE:

DISC OPERATING SYSTEM (SINGLE USER)
LOADER WITH OVERLAY FEATURES
FORTRAN COMPILER AND OBJECT TIME SYSTEM
DISPLAY SUBROUTINE PACKAGE
DIAGNOSTICS

THE DISC OPERATING SYSTEM PROVIDES THE BASE FOR THE REST OF THE SOFTWARE. IT PROVIDES DEVICE DRIVERS, A FILE SYSTEM AND OTHER PROGRAM SERVICES FOR A SINGLE USER. THE LOADER WITH OVERLAY CAPABILITIES ALLOWS LARGE PROGRAMS TO BE SEGMENTED FOR THE LIMITED MEMORY OF THE COMPUTER.

THE FORTRAN COMPILER AND OBJECT TIME SYSTEM PROVIDE THE SUPPORT FOR THE LANGUAGE IN WHICH MOST OF THE SOFTWARE IS WRITTEN. THE DISPLAY SUBROUTINE PACKAGE PROVIDES THE INTERFACE BETWEEN THE APPLICATIONS CODE AND THE DISPLAY.

THE OPERATING SYSTEM IS DEC DOS/BATCH VERSION 9. THIS OPERATING SYSTEM HAS NO PARTICULAR ADVANTAGE OVER SEVERAL OTHER CURRENT SYSTEMS, BUT WAS CHOSEN AS THE ONE SUITABLE SYSTEM AT THE TIME OF PURCHASE OF THE TERMINALS (JANUARY, 1973). THE MOST SERIOUS IMPACT OF SUBSTITUTING A DIFFERENT OPERATING SYSTEM WOULD BE ON THE COMMUNICATIONS CODE. MULTI-USER SYSTEMS COULD BE CONSIDERED, BUT WOULD PROBABLY REQUIRE EXTRA MEMORY AND MORE DISC CAPACITY THAN WE HAVE PROVIDED. THE CENTRAL SITE COMMUNICATIONS PROTOCOL IS NOT WELL SUITED TO UNATTENDED USE, AND THUS WOULD REQUIRE A FOREGROUND SLOT IN A MULTI-USER SYSTEM.

THE DOS/BATCH LOADER ALLOWS BOTH A SINGLE LEVEL MANUAL OVERLAY SCHEME, WHICH IS USED BY MOST OF THE PROGRAMS, AND AN AUTOLOAD SCHEME WHICH IS USED BY SOME. CONVERSION FROM ONE SCHEME TO THE OTHER CAN BE QUITE TEDIOUS BUT IS FEASIBLE.

THE FORTRAN COMPILER AND OBJECT TIME SYSTEM ARE DEC STANDARD PRODUCTS WITH A FEW SUBROUTINE CHANGES TO FACILITATE INPUT FROM THE KEYBOARD AND ASYNCHRONOUS INPUT/OUTPUT. CONVERSION TO ANOTHER COMPILER WOULD PROBABLY NOT REQUIRE SOURCE CODE OF THE COMPILER ITSELF, BUT WOULD VERY LIKELY REQUIRE SOURCE CODE AND SPECIFICATIONS OF THE OBJECT TIME SYSTEM. THE DISPLAY SUBROUTINE PACKAGE CHOSEN IS VECTOR GENERAL'S FORTRAN DRAWING PACKAGE VERSION 6. WE HAVE HAD MOST UNFORTUNATE EXPERIENCE WITH LATER VERSIONS OF THIS PACKAGE. SEVERAL SUBROUTINES IN THIS VERSION HAVE BEEN MODIFIED, WHICH MAKES CONVERSION DIFFICULT. ONE SHOULD CONSIDER ANY CHANGE AS REQUIRING AT LEAST TWO MAN-MONTHS OF EFFORT.

DIAGNOSTICS HAVE BEEN THOSE PROVIDED BY THE EQUIPMENT VENDORS. ONE MUST HAVE THESE ROUTINES IF ONE IS GOING TO RELY ON ANY SERVICE OTHER THAN THAT PROVIDED BY THE VENDOR, AND ONE IS WELL ADVISED TO OBTAIN THEM IN ANY CASE.

3. DETAILED HARDWARE CONFIGURATION

WE PRESENT A POSSIBLE CONFIGURATION FOR THE HARDWARE. PRICES WILL NOT BE INCLUDED SINCE THESE ARE CHANGING RAPIDLY AND ARE SUBJECT TO NEGOTIATION. AT THE TIME OF THIS WRITING, IT IS POSSIBLE TO ASSEMBLE SUCH A TERMINAL FOR ABOUT $100,000, INCLUDING SOFTWARE LICENSES.

WE WISH TO MAKE IT ABSOLUTELY CLEAR THAT, THOUGH WE WILL GIVE CONFIGURATIONS ONLY FOR THE VENDORS WITH WHICH WE HAVE DIRECT EXPERIENCE, THIS DOES NOT CONSTITUTE AN ENDORSEMENT OF THE PRODUCTS OF THESE VENDORS IN PREFERENCE TO ANY OTHERS. WE MERELY PRESENT A RANGE OF CONFIGURATIONS WHICH WE KNOW WILL DO THE JOB.

3.1. MINICOMPUTER

THE MINICOMPUTER IS A DEC PDP11/40-BS COMPUTER, WITH KE11-E EXTENDED INSTRUCTION SET, KE11-F FLOATING INSTRUCTION SET, KW11-L LINE FREQUENCY CLOCK, BM873-YB RESTART LOADER, RK11-DE DISC CARTRIDGE DRIVE, TM11-EA NINE-TRACK MAGNETIC TAPE TRANSPORT, AND DD11-A PERIPHERAL MOUNTING PANEL.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: 11/40-BS
PREREQUISITES: NONE STATUS: MANDATORY

DESCRIPTION: PDP-11/40 COMPUTER, 11/40 CENTRAL PROCESSOR WITH 28K 16 BIT WORD PARITY CORE MEMORY, LA36 DECWRITER AND CONTROL (DL11-A), CABINET.

ALTERNATIVES: 11/45-BW, 11/50-BW, 11/50-BS, OR OTHER MORE POWERFUL CPUS MAY BE SUBSTITUTED. COMMUNICATIONS CODE WILL RUN, BUT ALL FORTRAN CODE MUST BE RELINKED, AND PROBABLY SHOULD BE RECOMPILED.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: KE11-E
PREREQUISITES: 11/40 STATUS: MANDATORY

DESCRIPTION: EXTENDED INSTRUCTION SET (EIS) OPTION. PROVIDES EXTENDED MANIPULATION OF FIXED POINT NUMBERS, SIGNED INTEGER MULTIPLY AND DIVIDE, AND LONG SHIFTS.

ALTERNATIVES: THIS OPTION IS NEEDED TO ALLOW THE CPU TO KEEP UP WITH THE DISPLAY. IT IS NOT NEEDED FOR THE MORE POWERFUL CPUS.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: KE11-F
PREREQUISITES: KE11-E STATUS: MANDATORY

DESCRIPTION: FLOATING POINT OPTION. PROVIDES FLOATING POINT ADD, SUBTRACT, MULTIPLY, AND DIVIDE.

ALTERNATIVES: THIS OPTION IS NEEDED TO ALLOW THE CPU TO KEEP UP WITH THE DISPLAY. IT IS NOT NEEDED FOR THE MORE POWERFUL CPUS, WHICH TAKE INSTEAD THE FP11-B FLOATING POINT PROCESSOR. ONE MIGHT ALSO CONSIDER THE KE11-A EXTENDED ARITHMETIC ELEMENT, IF ONE IS CONSTRAINED TO USE ONE OF THE LESS POWERFUL CPUS.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: KW11-L
PREREQUISITES: 11/CPU STATUS: DESIRABLE

DESCRIPTION: LINE FREQUENCY REAL-TIME CLOCK.

ALTERNATIVES: ONE COULD OMIT THIS ITEM WITHOUT IMPACT ON THE SOFTWARE, EXCEPT THAT THE OPERATING SYSTEM COULD NOT TRACK THE TIME OF DAY. ONE CAN SUBSTITUTE A KW11-P, PROGRAMMABLE REAL-TIME CLOCK, OR HAVE BOTH IN THE SYSTEM.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: BM873-YB
PREREQUISITES: 11/CPU STATUS: DESIRABLE

DESCRIPTION: RESTART LOADER. CONTAINS ROM WITH BOOTSTRAP PROGRAM FOR PAPER TAPE, DISCS (RK11, RP11, RJS03, RJS04, RJP04) MAGNETIC TAPE (TU10, TU16), DECTAPE AND CASSETTE.

ALTERNATIVES: THIS OPTION ALLOWS ONE TO RESTART THE SYSTEM WITHOUT TEDIOUS ENTRY OF A BOOTSTRAP PROGRAM BY HAND. DEPENDING UPON THE DEVICES FROM WHICH ONE MIGHT WISH TO RESTART, ONE MIGHT CHOOSE THE MR11-DB (DISCS, DECTAPE, MAGTAPE) AND/OR BM792-YC (CARD READER). IF THE SYSTEM DOES NOT INCLUDE SUCH A LOADER, RESTART OF THE SYSTEM AFTER A CRASH SITUATION CAN BE QUITE TIME CONSUMING. THIS CAN BE TOLERATED IF ONE HAS PAPER TAPE EQUIPMENT AND PUTS THE OTHER BOOTSTRAPS ON PAPER TAPE.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: RK11-DE
PREREQUISITES: 11/CPU STATUS: MANDATORY

DESCRIPTION: 1.2 MILLION (16 BIT) WORD DISC CARTRIDGE DRIVE AND CONTROL UNIT. EXPANDABLE TO A TOTAL OF 8 RK05 DECPACK DISC DRIVES. 11 MICRO-SECONDS PER WORD TRANSFER RATE, 70 MSEC ACCESS TIME.

ALTERNATIVES: SIMILAR DISC SYSTEMS FROM OTHER VENDORS WHICH LOOK TO THE SYSTEM EXACTLY LIKE AN RK05 MAY BE SUBSTITUTED. LARGER DISC SYSTEMS SUCH AS THE RP11-CE MAY BE SUBSTITUTED HERE, BUT CAUTION MUST BE EXERCISED, AS NOT ALL THESE DISCS HAVE DRIVERS AVAILABLE FOR THE SYSTEM CHOSEN.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: TM11-EA
PREREQUISITES: 11/CPU STATUS: MANDATORY

DESCRIPTION: NINE-TRACK MAGNETIC TAPE TRANSPORT AND CONTROL UNIT. EXPANDS TO A TOTAL OF EIGHT TU10 TRANSPORTS (SEVEN OR NINE TRACK). 45 IN/SEC, 800 BPI NRZI.

ALTERNATIVES: THE SEVEN TRACK TM11-FA MAY BE USED INSTEAD, IF LOCAL REQUIREMENTS MAKE THIS DESIRABLE. DRIVES FROM OTHER VENDORS WHICH APPEAR IDENTICAL TO THE SOFTWARE MAY ALSO BE SUBSTITUTED.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: DD11-A
PREREQUISITES: 11/CPU STATUS: MANDATORY

DESCRIPTION: PERIPHERAL MOUNTING PANEL. A PREWIRED SYSTEM UNIT DESIGNED FOR MOUNTING UP TO FOUR SMALL PERIPHERAL CONTROLLER (SPC) INTERFACES.

ALTERNATIVES: THIS ITEM IS NEEDED FOR THE CONFIGURATION GIVEN, TO ALLOW INSTALLATION OF THE PERIPHERALS FROM OTHER VENDORS. IF EVEN MORE PERIPHERALS ARE CHOSEN, A BA11-ES EXTENSION MOUNTING BOX AND H720 POWER

SUPPLY PLUS BUS CABLE MAY WELL BE NEEDED. ONE MAY ALSO NEED AN EXTRA H960 CABINET.

3.2. DISPLAY SYSTEM

THE DISPLAY SYSTEM IS A VECTOR GENERAL 3D2 DISPLAY SYSTEM, WITH CD1 CONTROL DIALS, AD1 A TO D CONVERTER WITH 8 CHANNEL MULTIPLEXER, MX1 ADDITIONAL EIGHT-CHANNEL MULTIPLEXER, DI2 ANALOG DEVICE INTERFACE, IM1 INTENSITY MODULATION FEATURE, DEC1 PDP11 INTERFACE, SS1 SUBROUTINE-STACK FACILITY, AND PP1 PHOSPHOR PROTECT CIRCUIT.

VENDOR: VECTOR GENERAL, INC. ITEM: 3D2
PREREQUISITES: DEC1 STATUS: MANDATORY

DESCRIPTION: HIGH RESOLUTION DISPLAY SYSTEM WITH THREE-DIMENSIONAL ROTAION AND TRANSLATION. THIS IS A RANDOM DRAW SYSTEM, WITH A REFRESH DISPLAY CAPABLE OF SHOWING ABOUT 6000 STROKES WITH 4096 BY 4096 RESOLUTION.

ALTERNATIVES: THE EVANS AND SUTHERLAND PICTURE SYSTEM PROVIDES A VIABLE ALTERNATIVE, WITH SIMILAR FEATURES AND SLIGHTLY GREATER FLEXIBILTY. A SMALL STORAGE DISPLAY, SUCH AS THE TECTRONIX 4010, WOULD OFFER GREATLY REDUCED CAPABILITIES. THERE ARE MANY DISPLAYS BETWEEN THESE EXTREMES. A CHANGE TO ANY OF THESE WILL REQUIRE SIGNIFICANT PROGRAMMING EFFORT TO DEVELOP INTERFACE ROUTINES, UNLESS THE VENDOR PROVIDES ROUTINES OF CAPABILITY SIMILAR TO THOSE USED HERE. THE APPLICATIONS CODE WILL HAVE TO BE CHANGED SOMEWHAT, SINCE ROTATION MATRICES ARE TRANSMITTED VIA COMMON BLOCKS FOR MAXIMAL SPEED, AND THE DISPLAY SCALING ROUTINES ARE USED, SO THAT A PICTURE SPACE IN THE RANGE FROM -20.48 TO +20.48 IS ASSUMED. VECTOR GENERAL NOW OFFERS A 3D3 SYSTEM, WHICH IS COMPATIBLE, BUT IS SOMEWHAT FASTER.

VENDOR: VECTOR GENERAL, INC. ITEM: CD1
PREREQUISITES: AD1,MX1 STATUS: MANDATORY

DESCRIPTION: CONTROL DIALS. CONSISTS OF TEN MANUALLY-OPERATED DIALS THAT ARE USED FOR SENDING NUMERICAL DATA TO THE COMPUTER FOR USE UNDER PROGRAM CONTROL.

ALTERNATIVES: THESE DIALS ARE USED BY THE APPLICATIONS CODE FOR SUCH FEATURES AS DYNAMIC CONTROL OF ORIENTATION. WITHOUT THEM, ONE WOULD BE OBLIGED TO TYPE IN NUMBERS FROM THE KEYBOARD, SEVERELY DEGRADING THE REAL-TIME CHARACTERISTICS OF THE CODE. ONE COULD SUBSTITUTE ALMOST ANY ANALOG TO DIGITAL SYSTEM WITH TEN 12-BIT INPUTS.

VENDOR: VECTOR GENERAL, INC. ITEM: AD1
PREREQUISITES: DI2 STATUS: MANDATORY

DESCRIPTON: ANALOG TO DIGITAL CONVERTER WITH EIGHT-CHANNEL MULTIPLEXER.

ALTERNATIVES: THIS CONVERTER SUPPORTS THE CONTROL DIALS. IF AN ALTERNATE DEVICE IS USED, THE CONVERTER MAY NOT BE NEEDED.

VENDOR: VECTOR GENERAL, INC. ITEM: MX1
PREREQUISITES: AD1 STATUS: MANDATORY

DESCRIPTION: ADDITIONAL EIGHT-CHANNEL MULTIPLEXER.

ALTERNATIVES: LEAVING THIS OUT WOULD DISABLE FIVE OF THE DIALS IN CD1.

VENDOR: VECTOR GENERAL, INC. ITEM: DI2
PREREQUISITES: 3D2 STATUS: MANDATORY

DESCRIPTION: ANALOG DEVICE INTERFACE

ALTERNATIVES: IF THE DIALS ARE NOT NEEDED, THIS MAY BE OMITTED ALSO.

VENDOR: VECTOR GENERAL, INC. ITEM: IM1
PREREQUISITES: 3D2 STATUS: OPTIONAL

DESCRIPTION: INTENSITY MODULATION. PROVIDES DEPTH SIMULATION BY VARIATION OF THE INTENSITY OF THE Z-AXIS DRAW. ALSO PROVIDES A PLANE CUTOFF WHICH ALLOWS CONTROLLED REMOVAL OF FIGURE SECTIONS.

ALTERNATIVES: THIS FEATURE GREATLY ENHANCES THE REALITY OF A DRAWN MODEL. FOR VIEWERS WHO ARE ESPECIALLY ADEPT AT VIEWING STEREO PAIRS, IT MIGHT NOT BE NECESSARY TO HAVE THIS FEATURE.

VENDOR: VECTOR GENERAL, INC. ITEM: DEC1
PREREQUISITES: 11/CPU STATUS: MANDATORY

DESCRIPTION: INTERFACE TO COMPUTER. PROVIDES BOTH PROGRAMMED AND DMA TRANSFERS TO THE DISPLAY.

ALTERNATIVES: A NEWER INTERFACE IS AVAILABLE WITH ITS OWN REFESH BUFFER MEMORY. USE OF THIS INTERFACE WOULD GREATLY REDUCE THE CPU LOAD. IT WOULD REQUIRE CHANGES IN THE DRIVING SOFTWARE, BUT NOT IN THE APPLICATIONS CODE. ABOUT TWO MAN-WEEKS OF PROGRAMMER TIME WOULD SUFFICE FOR THE CHANGES.

VENDOR: VECTOR GENERAL, INC. ITEM: SS1
PREREQUISITES: DEC1 STATUS: DESIRABLE

DESCRIPTION: SUBROUTINE STACK FACILITY. ALLOWS DISPLAY LIST CONTROL OF DIRECT DATA TRANSFER BETWEEN THE DISPLAY CONTROLLER AND THE PROCESSOR AND DIRECT GRAPHIC SUBROUTINING.

ALTERNATIVES: THIS FEATURE IS NOT HEAVILY USED BY THE APPLICATIONS SOFTWARE AT PRESENT. IF ONE WISHES TO PUSH THE DISPLAY FOR MAXIMUM IMAGE COMPLEXITY, IT IS BEST TO TAKE THIS OPTION.

VENDOR: VECTOR GENERAL, INC ITEM: PP1
PREREQUISITES: 3D2 STATUS: DESIRABLE

DESCRIPTION: PHOSPHOR PROTECT CIRCUIT. IF DEFLECTION IS NOT PROVIDED, THE DISPLAY IS BLANKED TO AVOID BURNING A HOLE IN THE SCREEN.

3.3 COMMUNICATIONS GEAR

THE COMMUNICATIONS GEAR IS A DEC DU11 WITH SANGAMO TA201A/B3/4S MODEM, AND DEC DL11-E WITH OMNITEC 702A1 TELEPHONE COUPLER.

VENDOR: SANGAMO ELECTRIC COMPANY ITEM: TA201A/B3/4S
PREREQUISITES: DP11 OR DU11 STATUS: MANDATORY

DESCRIPTION: MODEM FOR SYNCHRONOUS, SERIAL, BINARY DATA AT 2000 BAUD. CONNECTS TO THE DIRECT DISTANCE DIALING NETWORK VIA A CDT DIRECT ACCESS ARRANGEMENT.

ALTERNATIVES: THERE ARE MANY VENDORS OF EQUIVALENT MODEMS. ONE MUST BE CERTAIN THAT THE MODEM IS FOR HALF-DUPLEX 2000 BAUD USE OVER THE DIRECT DISTANCE DIALING NETWORK IN A MANNER COMPATIBLE WITH WESTERN ELECTRIC 201A DATA SETS. ONE MUST BE CERTAIN THAT AN INTERFACE TO THE TELEPHONE LINES IS AVAILABLE FOR THE MODEM CHOSEN. A GOOD PRACTICE IS TO RENT A DATA SET FROM THE TELEPHONE COMPANY WHILE GETTING STARTED, AND THEN PURCHASE A MODEM AFTER EVERYTHING IS WORKING WELL. THE MODEM CHOSEN MUST HAVE A STANDARD EIA RS232C INTERFACE TO WORK WITH THE DP11 OR DU11.

IF ONE WISHES TO WORK WITH A COMPUTER CENTER THAT HAS DEDICATED LINES OR HIGHER SPEED DIAL-UP MODEMS, ONE MUST USE A MODEM SPECIFIED BY THE CENTER. PRESENT SOFTWARE HAS BEEN USED WITH DEDICATED LINES AT SPEEDS OF UP TO 9600 BAUD.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: DU11-DA
PREREQUISITES: 11/CPU STATUS: MANDATORY

DESCRIPTION: CONTROL FOR SYNCHRONOUS MODEM.

ALTERNATIVES: THE OLDER DP11-DA CAN BE USED INSTEAD. SOFTWARE IS NOT PROVIDED FOR THE DQ11-DA OR DV11-DA SYNCHRONOUS INTERFACES. IF THESE ARE USED, ONE WOULD HAVE TO INVEST ON THE ORDER OF TWO MAN-WEEKS TO PROVIDE CODE FOR THE PROTOCOL.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: DL11-E
PREREQUISITES: 11/CPU STATUS: DESIRABLE

DESCRIPTION: CONTROL FOR ASYNCHRONOUS MODEM. ONE MUST SPECIFY THE DESIRED BAUD RATE. A RATE OF 300 BAUD IS SUITABLE FOR MOST CENTERS, BUT NOT FOR ALL. THE RANGE OF RATES ALLOWED IS CONTROLLED BY A CRYSTAL ON THE BOARD. GROUP 4 ALLOWS 300 BAUD AND SPEEDS UP TO 9600 BAUD. GROUP 3 DOES NOT ALLOW SUCH HIGH SPEEDS, BUT INCLUDES 1800 BAUD, WHICH SUITS SOME CENTERS.

ALTERNATIVES: THIS OPTION IS USEFUL WHEN COMMUNICATING WITH CENTERS WHICH DO NOT PROVIDE THE SYNCHRONOUS PROTOCOL REQUIRED, BUT WHICH DO HAVE KEYBOARD TERMINAL LINES. SOFTWARE IS AVAILABLE TO MAKE THE TERMINAL APPEAR AS A SIMPLE TECTRONIX 4010.

VENDOR: OMNITEC CORPORATION ITEM: 702A1
PREREQUISITES: DL11 STATUS: DESIRABLE

DESCRIPTION: ASYNCHRONOUS MODEM WITH ACOUSTIC AND DAA TELEPHONE COUPLER.

ALTERNATIVES: THERE ARE MANY ALTERNATIVE MODEMS FOR ASYNCHRONOUS USE. FOR MOST CENTERS, ONE WANTS 300 BAUD (30 CHARACTERS PER SECOND) CAPABILITY. FOR SOME CENTERS, ONE WOULD LIKE 1200 BAUD, OR 1800 BAUD CAPABILITY. BE CERTAIN THE MODEM CHOSEN MATCHES THE CENTER. THIS MODEM INCLUDES ANSWER AS WELL AS ORIGINATE CAPABILITY. BE CERTAIN TO TAKE ONE WITH THIS FEATURE IF YOU WISH TO USE THE MODEM TO SUPPORT AN INCOMING TERMINAL.

3.4. PRINTER/PLOTTER

VENDOR: VERSATEC ITEM: C-PDP11 (DMA)
PREREQUISITES: 11/CPU STATUS: MANDATORY

DESCRIPTION: THIS IS A CONTROLLER FOR THE VERSATEC MATRIX 1100A PRINTER/PLOTTER. IT PROVIDES BOTH BYTE BY BYTE AND DMA DATA TRANSFERS TO THE DEVICE, USING REGISTERS SIMILAR TO THE DEC LP11 FOR THE PRINTER.

ALTERNATIVES: THE NON-DMA CONTROLLER MAY BE USED, SINCE NONE OF THE SOFTWARE ACTUALLY USES THE DMA LOGIC. THIS LIMITS ONE ONLY IN TERMS OF FUTURE EXPANSION OF CODE REQUIRING FASTER TRANSFERS WITH LESS CPU LOAD. IF ONE TAKES THE DEC LV11 INTERFACE, THE PLOT DRIVER WILL HAVE TO BE REVISED (ABOUT ONE MAN-WEEK). IF ONE TAKES A COMPLETELY DIFFERENT VENDOR'S DEVICE, ABOUT TWO MAN-WEEKS WILL BE REQUIRED FOR NEW DRIVERS, AND ABOUT TWO MAN-WEEKS FOR APPLICATIONS CODE, IF THE PAGE LAYOUT IS DIFFERENT.

VENDOR: VERSATEC ITEM: MATRIX 1100A
PREREQUISITES: C-PDP11 (DMA) STATUS: MANDATORY

THIS IS AN ELECTROSTATIC PRINTER/PLOTTER. IT PRINTS AT 500 LINES PER MINUTE ON 11 BY 8 1/2 INCH FAN-FOLD PAPER. IT PRINTS 132 CHARACTERS PER LINE. IT PLOTS 100 DOTS TO THE INCH, WITH 1024 DOTS ACROSS A PAGE AT

1.2 INCHES PER SECOND SCAN RATE.

ALTERNATIVES: THERE ARE MANY MODELS OF THIS DEVICE, AND SEVERAL ALTERNATE VENDORS. MUCH OF THE SOFTWARE ASSUMES THE AVAILABILITY OF A PRINTER. IT IS POSSIBLE TO DO SUCH PRINTING ON THE CONSOLE DEVICE, BUT MOST CONSOLE DEVICES ARE TOO SLOW FOR ANY QUANTITY OF DATA. HOWEVER, IF MONEY IS TIGHT, AND SOMETHING MUST GO, ONE CAN TAKE JUST THE PLOT LOGIC, AND MAKE A SOFTWARE CHARACTER GENERATOR. THE PLOT CAPABILITY IS ESSENTIAL TO THE GRAPHICS IN ORDER TO GET HARD COPY. ONE COULD SUBSTITUTE A CAMERA, BUT SUPPLY COSTS THEN RUN VERY HIGH. IF ONE TAKES A DIFFERENT VENDOR'S DEVICE, IT SHOULD BE NOTED THAT THE SOFTWARE OFTEN ASSUMES 132 CHARACTER LINES, AND 100 DOTS TO THE INCH PLOTTING ON 1024 DOT WIDE RASTERS. IT WOULD TAKE ABOUT TWO MAN-WEEKS TO GO THROUGH THE APPLICATIONS CODE AND CHANGE TO ANOTHER PATTERN. IT WOULD TAKE ABOUT TWO MAN-WEEKS TO WRITE A DRIVER FOR A DIFFERENT DEVICE.

3.5. CARD READER

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: CR11
PREREQUISITES: 11/CPU STATUS: DESIRABLE

DESCRIPTION: PUNCHED CARD READER AND CONTROL UNIT. 300 CARDS/MINUTE.

ALTERNATIVES: ANY SUITABLE UNIT RECORD PERIPHERAL SUPPORTED BY THE HOST SYSTEM MAY BE USED TO MEET LOCAL REQUIREMENTS. THE MAIN CONSIDERATION IS THE AVAILABILITY OF AUXILIARY EQUIPMENT TO PREPARE INPUT FOR THE SYSTEM. THUS IF CARD KEY-PUNCHES ARE AVAILABLE, ONE SHOULD TAKE A CARD READER. IT SHOULD BE NOTED THAT A CARD READER DRIVER FOR THE CR11 HAS BEEN MODIFIED TO ALLOW USE OF THE CDC 026 CHARACTER SET, AND TO ALLOW USE OF ASCII 256 CODE FOR BINARY INPUT. IF THESE FEATURES ARE DESIRED, AND ANOTHER CARD READER IS CHOSEN, THE DRIVER FOR THAT READER WILL HAVE TO BE ALTERED. THIS WOULD REQUIRE ABOUT ONE MAN-WEEK OF PROGRAMMING EFFORT.

4. DETAILED SOFTWARE CONFIGURATION

4.1. DISC OPERATING SYSTEM

THE DISC OPERATING SYSTEM, LOADER WITH OVERLAY FEATURES, AND FORTRAN COMPILER WITH OBJECT TIME SYSTEM WERE ALL OBTAINED AS PART OF THE DOS/BATCH-11 OPERATING SYSTEM.

VENDOR: DIGITAL EQUIPMENT CORP. ITEM: QJ250-AD
PREREQUISITES: 11/CPU, 16K MEM, RK11, TM11
STATUS: MANDATORY

DESCRIPTION: DOS/BATCH-11. THIS IS BOTH A KEYBOARD ORIENTED PROGRAM DEVELOPMENT SYSTEM, AND A BATCH ORIENTED JOB PROCESSING SYSTEM. IT CONTAINS MONITOR, EDITOR, MACRO ASSEMBLER, LINKER, LIBRARIAN, DEBUGGING TOOL, PERIPHERAL INTERCHANGE PROGRAM FILE UTILITY, FORTRAN IV COMPILER AND OBJECT TIME SYSTEM, FILE COMPARE, VERIFY, AND DUMP PROGRAMS, AND OTHER UTILITIES. THIS IS THE NINE-TRACK MAGTAPE RELEASE. OTHER MEDIA ARE AVAILABLE.

ALTERNATIVES: VERSION 9 OF THIS SYSTEM IS KNOWN TO SUPPORT THE CRYSNET SOFTWARE. IF ANOTHER COMPUTER IS USED, ONE MUST OF COURSE OBTAIN SOFTWARE FOR THAT MACHINE. IF THE SAME TYPE OF COMPUTER IS CHOSEN, BUT APPLICATIONS MANDATE FEATURES NOT FOUND IN THIS SYSTEM, ONE HAS A WIDE RANGE OF AVAILABLE SYSTEMS FROM WHICH TO CHOOSE. THE COMMUNICATIONS SOFTWARE AND THE DISPLAY SUPPORT CODE ARE THE MOST DIFFICULT TO CONVERT. THE COMMUNICATIONS CODE IS IN ASSEMBLY LANGUAGE, AND ASSUMES THE FILE SYSTEM CONVENTIONS OF DOS/BATCH. THE STANDARD DOS/BATCH KEYBOARD DRIVER HAS BEEN REPLACED TO ALLOW KEYBOARD INPUT TO BE PENDING WHILE MESSAGES ARE PRINTED OUT. ABOUT FOUR MAN-MONTHS FOR CONVERSION WOULD BE REQUIRED. THE SOFTWARE SYSTEM FOR THE DISPLAY IS ALSO IN ASSEMBLY LANGUAGE, BUT HAS FORTRAN EQUIVALENTS IN LARGE PART. THE ACTUAL DEVICE DRIVING CODE DOES NOT CONFORM TO DOS/BATCH CONVENTIONS, AND THUS REQUIRES ACCESS TO THE DISPLAY DIRECTLY FROM THE USER PROGRAM. THIS WOULD CAUSE SOME DIFFICULTY IN A SYSTEM WITH MEMORY PROTECTION IN USE. FOR FURTHER COMMENTS ON THE DISPLAY SOFTWARE, SEE BELOW.

THE FORTRAN OBJECT TIME SYSTEM HAS BEEN MODIFIED TO INCLUDE AN ASYNCHRONOUS INPUT/OUTPUT FEATURE (BUFFEI/BUFFEO), WHICH ALLOWS A DISPLAY PROGRAM TO RUN WHILE WAITING FOR KEYBOARD INPUT. USE OF ANOTHER OPERATING SYSTEM OR DIFFERENT LEVEL OF THE FORTRAN COMPILER WOULD REQUIRE EITHER A CHANGE IN THE DISPLAY PROGRAMS, OR REINTRODUCTION OF THIS FEATURE, OR USE OF AN EQUIVALENT FEATURE. ABOUT TWO MAN-WEEKS SHOULD BE ALLOWED FOR SUCH A CHANGE.

FURTHER, THE FORMAT SPECIFICATION INTERPRETER HAS BEEN MODIFIED TO ALLOW TERMINATION OF NUMERIC INPUT FIELDS BY COMMAS, AND TO ALLOW A B-FORMAT SPECIFICATION FOR SIMILARLY TERMINATED ALPHANUMERIC INPUT. PART OF THIS FEATURE WAS ADOPTED BY DEC, BUT NOT ALL OF IT, SO AGAIN USE OF A DIFFERENT SYSTEM, OR VERSION OF THE SAME SYSTEM, WOULD IMPLY A CONVERSION EFFORT. HOWEVER, IN THIS CASE ONE COULD LIVE WITHOUT THE FEATURES AT THE EXPENSE OF MORE CUMBERSOME INPUT TO THE PROGRAMS. ALL THAT IS REQUIRED IS TO EDIT OUT ALL B-FORMAT SPECIFICATIONS AND REPLACE THEM WITH A-FORMAT SPECIFICATIONS. ABOUT ONE MAN-WEEK SHOULD BE ALLOWED FOR THIS TASK.

4.2. DISPLAY SUBROUTINE PACKAGE

VENDOR: VECTOR GENERAL, INC. ITEM: FDP-6
PREREQUISITES: QJ250, 302, DEC1 STATUS: MANDATORY

DESCRIPTION: FORTRAN DRAWING PACKAGE. THIS IS A COLLECTION OF SUBROUTINES TO ALLOW FORTRAN PROGRAMS ON A DEC PDP11 TO GENERATE AND MODIFY PICTURES ON A VECTOR GENERAL DISPLAY SYSTEM.

ALTERNATIVES: FOR DIFFERENT HARDWARE, THE CREATION OF AN EQUIVALENT PACKAGE ABLE TO SUPPORT THE CRYSNET PROGRAMS SHOULD TAKE ABOUT FOUR MAN-MONTHS. ON THE SAME HARDWARE, IT IS NOT REASONABLE TO TAKE OR CREATE A DIFFERENT PACKAGE, OR EVEN A DIFFERENT VERSION OF THE SAME PACKAGE, UNLESS FORCED TO DO SO. IN PARTICULAR, IT HAS NOT BEEN POSSIBLE TO GET RELIABLE OPERATION OF THE SOFTWARE WITH RELEASE 7 OF THE SAME PACKAGE. IF SUPPORT FOR SPECIAL FEATURES REQUIRES ONE TO TAKE SUCH A PACKAGE, ABOUT TWO MAN-MONTHS FOR CLEAN-UP AND CONVERSION SHOULD BE ALLOWED. ONE MIGHT ALSO WISH TO TAKE THE FILE MANAGEMENT PACKAGE (FMP), THOUGH THE EXISTING SOFTWARE DOES NOT NEED IT.

4.3. DIAGNOSTICS

FOR EACH DEVICE PURCHASED, ONE NORMALLY RECEIVES A DIAGNOSTIC PROGRAM. IN SOME CASES, THE VENDOR MAY REQUIRE EXPLICIT SPECIFICATION OF THIS REQUIREMENT IN ORDER TO DELIVER THE ITEM. SINCE IT IS COMMON TO PROVIDE SUCH DIAGNOSTICS ON PAPER TAPE, AND THE CONFIGURATION GIVEN DOES NOT INCLUDE A PAPER TAPE READER, ONE MUST REQUEST A COPY EITHER ON CARDS OR MAGNETIC TAPE. IF THE ABOVE CONFIGURATION IS USED, AND THE DIAGNOSTICS ARE WRITTEN AS DOS FORMAT BINARY FILES, A UTILITY IS AVAILABLE TO LOAD THE DIAGNOSTICS.

5. SUPPLIES

A TERMINAL SUCH AS SPECIFIED HERE CONSUMES LARGE QUANTITIES OF SUPPLIES. IT IS NOT POSSIBLE TO GIVE EXACT QUANTITIES, SINCE THESE DEPEND UPON ACTUAL PATTERNS OF USE. SUFFICE IT TO SAY THAT ONE MUST ARRANGE TIMELY DELIVERY OF

PAPER FOR PRINTER/PLOTTER
TONER AND DISPERSANT FOR PRINTER/PLOTTER
PAPER FOR CONSOLE DEVICE (IF HARDCOPY)
RIBBONS FOR CONSOLE DEVICE (IF HARDCOPY)
MAGNETIC TAPES
DISC PACKS

IF EXTRA DEVICES ARE ADDED, SUCH AS PAPER TAPE EQUIPMENT, SUPPLIES MAY WELL BE NEEDED FOR THEM. THERE ARE ALTERNATE VENDORS FOR MOST OF THE ITEMS REQUIRED, AND ONE IS WELL ADVISED TO VERIFY RESPONSE TIME TO DELIVERY REQUESTS, SINCE IT IS POOR PRACTICE TO STOCK TOO HEAVILY IN-HOUSE. THIS IS ESPECIALLY TRUE FOR THE PAPER FOR THE PRINTER/PLOTTER WHICH CANNOT BE USED IF STORED FOR TOO LONG OR UNDER IMPROPER CONDITIONS. ONE CAN EASILY USE 1000 SHEETS OF THIS PAPER A WEEK, SO A PURCHASE OF A DOZEN BOXES PER QUARTER WOULD BE A FAIR ESTIMATE FOR THE FIRST YEAR. WITH THAT SORT OF A LOAD, ONE COULD USE SIX BOTTLES OF TONER FOR THE YEAR. WITH OTHER SUPPLIES, $2000 IS A FAIR BUDGET FOR SUPPLIES FOR THE FIRST YEAR, IF NO OTHER EXPERIENCE IS AVAILABLE TO MAKE AN ESTIMATE. THE VARIANCE OF THIS NUMBER IS VERY LARGE.

6. MAINTENANCE

ONE MUST ARRANGE TO HAVE THE EQUIPMENT MAINTAINED. THERE IS NO WAY TO AVOID THIS EXPENSE. IF ONE DOES NOTHING, DEVICES WILL FAIL SO BADLY AS TO REQUIRE TOTAL REPLACEMENT. IF ONE PERFORMS MAINTENANCE IN-HOUSE, ONE MUST INVENTORY SPARES, TRAIN PEOPLE, AND PAY SALARIES. IF ONE USES VENDORS, ONE MUST PAY FOR THEIR SERVICES. BY ANY TECHNIQUE, MAINTENANCE ON EQUIPMENT OF THE TYPE CONSIDERED HERE COSTS AN AVERAGE OF ABOUT 10 PER CENT OF THE PURCHASE PRICE PER YEAR. THIS PRICE GOES UP IF ONE REQUIRES VERY FAST REPAIRS, AND GOES DOWN IF ONE CAN STAND LONG DELAYS.

MAINTENANCE CONSISTS OF THREE MAJOR SERVICES

EMERGENCY MAINTENANCE
PREVENTIVE MAINTENANCE
ENGINEERING CHANGES

ALL OF THESE ARE NEEDED IN SOME FORM.

6.1. EMERGENCY MAINTENANCE

WHEN SOMETHING BREAKS, ONE WISHES TO HAVE IT REPAIRED. ONE CAN EITHER SHIP IT TO THE PERSONS WHO WILL DO THE WORK, OR HAVE THEM COME TO THE EQUIPMENT. SHIPPING EQUIPMENT IS USUALLY SLOW AND CHEAP. SHIPPING PEOPLE IS USUALLY FAST AND EXPENSIVE. IT IS NOT REASONABLE TO SHIP ESPECIALLY HEAVY OR DELICATE EQUIPMENT, EXCEPT IN CASE OF VERY EXTENSIVE REPAIRS. IN ANY EVENT, MOST PEOPLE CANNOT ALLOW THE LONG DOWN PERIODS WHICH ARISE UPON RETURN OF EQUIPMENT FOR REPAIR, AND THUS WISH TO ARRANGE TO HAVE SERVICE PEOPLE COME TO THEM.

ONE CAN ARRANGE TO HAVE SERVICE PEOPLE COME EITHER ON AN 'ON-CALL' BASIS, OR ON A 'SERVICE CONTRACT' BASIS. IN ON-CALL SERVICE, ONE PAYS THE ACTUAL COSTS OF EACH CALL. WITH A SERVICE CONTRACT, ONE PAYS A FLAT RATE. MOST VENDORS TEND TO GIVE PRIORITY TO SERVICE FOR CUSTOMERS ON SERVICE CONTRACT. OUR EXPERIENCE HAS BEEN THAT SUCH CONTRACTS ARE OFTEN THE ONLY WAY TO OBTAIN LIMITED DOWN TIME. IT IS USUALLY POSSIBLE TO HAVE A CONTRACT WRITTEN WITH PENALTIES FOR FAILURE TO RESPOND WITHIN A GIVEN PERIOD, AND MOST SUCH CONTRACTS COVER PARTS AND LABOR FOR EVEN THE MOST CATASTROPHIC FAILURES.

6.2. PREVENTIVE MAINTENANCE

AS EQUIPMENT IS USED, VARIOUS PARTS BECOME DIRTY, WORN, ELECTRICALLY MARGINAL, OR OTHERWISE IN NEED OF ADJUSTMENT. RATHER THAN WAIT FOR TOTAL FAILURE, IT IS GOOD PRACTICE PERIODICALLY TO CLEAN PARTS, CHECK FOR WEAR, AND RUN DIAGNOSTICS. THE USER CAN, AND SHOULD DO SOME OF THIS HIMSELF. HOWEVER, MOST SERVICE CONTRACTS INCLUDE PREVENTIVE MAINTENANCE, AND EVEN IF ONE IS ON-CALL, IT IS WISE TO BRING IN THE SERVICE PEOPLE PERIODICALLY TO CHECK OUT THE EQUIPMENT CAREFULLY.

THE USER HIMSELF SHOULD ASSUME RESPONSIBILITY FOR CLEANING TAPE DRIVES BEFORE EACH USE, THE PRINTER/PLOTTER ON EACH PAPER CHANGE, AND THE FILTER ON THE VECTOR GENERAL DISPLAY EACH MONTH. THIS LATTER ITEM CAN CAUSE REALLY SERIOUS PROBLEMS IF NEGLECTED.

6.3. ENGINEERING CHANGES

THERE IS ALSO NEED AT TIMES TO UPGRADE EQUIPMENT. THIS IS DONE FOR SEVERAL REASONS. MAINTENANCE IS EASIER FOR A SERVICE ORGANIZATION IF ALL THE EQUIPMENT TO BE HANDLED IS ON THE SAME LEVEL. PROBLEMS WHICH CAUSE FREQUENT FAILURES CAN OFTEN BE REMEDIED BY GOING TO A LATER VERSION OF THE HARDWARE. DEVICE PERFORMANCE MAY BE IMPROVED. HARDWARE MAY BE MADE COMPATIBLE WITH OTHER, NEWLY INTRODUCED HARDWARE AND SOFTWARE. MAINTENANCE CONTRACTS OFTEN INCLUDE SOME SUCH UPGRADES, WITH THE REST AVAILABLE FOR AN EXTRA FEE. THE USER MUST ASSUME RESPONSIBILITY FOR EVALUATING THE DESIRABILITY OF EACH SUCH CHANGE, SINCE THESE CAN OFTEN INTRODUCE NEW PROBLEMS. HOWEVER IT IS DIFFICULT TO AVOID SUCH CHANGES FOREVER, AND IT IS WISE TO SCHEDULE THEM AT SOME STEADY RATE IN CONSULTATION WITH THE SERVICE ORGANIZATION.

7. POWER, ENVIRONMENTAL CONTROL, IN-HOUSE SUPPORT

IN ORDER TO RUN A TERMINAL SUCH AS THAT SPECIFIED HERE, ONE MUST HAVE ADEQUATE ELECTRICAL POWER, ENVIRONMENTAL CONTROL, AND IN-HOUSE SUPPORT. THE EXACT CONFIGURATION WILL DETERMINE THE POWER NEEDED. IF ONE USES PRECISELY THE EQUIPMENT GIVEN, THEN ONE NEEDS TWO SINGLE PHASE, 117 VOLT, 30 AMP CIRCUITS, AND ONE SINGLE PHASE 117 VOLT, 20 AMP CIRCUIT, AS AN ABSOLUTE MINIMUM FOR THE EQUIPMENT. OTHER OUTLETS WILL BE NEEDED IN THE SAME ROOM FOR TEST EQUIPMENT AND LIGHTS. THE ENVIRONMENTAL CONTROL WILL AGAIN DEPEND ON THE EXACT CONFIGURATION, BUT ONE WOULD DO BEST TO ALLOW 30,000 BTU PER HOUR HEAT LOAD IN A ROOM HELD AT 20 DEGREES CENTIGRADE, PLUS OR MINUS ONE DEGREE CENTIGRADE, WITH 40 TO 60 PER CENT RELATIVE HUMIDITY. FOR IN-HOUSE SUPPORT, ONE REQUIRES SOME RESPONSIBLE PERSON TO ACCEPT THE BURDEN OF MANAGING THE USE AND MAINTENANCE OF THE EQUIPMENT. ONCE IT IS INSTALLED, THIS SHOULD REQUIRE NO MORE THAN 20 PER CENT OF HIS TIME. THIS DOES NOT INCLUDE THE TIME OF IN-HOUSE REPAIR PEOPLE, IF THEY ARE USED. THE SYSTEM MANAGER WILL HAVE A MUCH HEAVIER BURDEN WHEN THE SYSTEM IS BEING PURCHASED AND INSTALLED. ALL SUCH ARRANGEMENTS, FOR POWER, ENVIRONMENTAL CONTROL, AND IN-HOUSE SUPPORT, SHOULD BE MADE WITH THE HELP OF THE ACTUAL EQUIPMENT VENDORS.

8. PURCHASE, INSTALLATION, AND ACCEPTANCE

THE MOST TIME-CONSUMING EFFORT IN OBTAINING SUCH A TERMINAL IS THE PERIOD OF ACTUAL PURCHASE, INSTALLATION AND ACCEPTANCE OF THE HARDWARE AND SOFTWARE. ONE MUST, OF COURSE COMPLY WITH THE REGULATIONS OF ONE'S INSTITUTION AND FUNDING AGENCIES IN BUYING SUCH EQUIPMENT. ONE FACES THE DIFFICULT CHOICE OF GOING OUT FOR BIDS, OR JUSTIFYING A SOLE-SOURCE AQUISITION. WE CANNOT SETTLE THIS QUESTION HERE. HOWEVER, ONE SHOULD BE CERTAIN TO MAKE CLEAR THAT ONE IS BUYING A FUNCTIONAL SYSTEM, NOT A COLLECTION OF PARTS. THUS ONE SHOULD INCLUDE IN THE PURCHASE SPECIFICATIONS OF EACH COMPONENT, THE REQUIREMENT THAT IT FUNCTION WITHIN THE SYSTEM AS A WHOLE. IF ONE IS NOT IN A POSITION TO DO SOFTWARE CONVERSIONS OF GREAT MAGNITUDE, THEN ONE MUST REQUIRE THAT THE SYSTEM RUN THE PORTIONS OF THE EXISTING SOFTWARE NECESSARY FOR THE APPLICATION AT HAND. IF ONE IS NOT IN A POSITION TO UNDERTAKE MAJOR MAINTENANCE IN-HOUSE, THEN ONE MUST, AT THE TIME OF PURCHASE, INSIST UPON THE AVAILABILITY OF ADEQUATE VENDOR MAINTENANCE AT AN AGREED PRICE. FURTHER, AT THE TIME OF PURCHASE ONE MUST MAKE ARRANGEMENTS TO INSTALL THE EQUIPMENT AND SYSTEM SOFTWARE. THE PRICE ONE PAYS FOR THIS SERVICE APPEARS HIGH, BUT IS WELL WORTH IT, SINCE ONE MUST OFTEN CONTRACT FOR THIS SERVICE IN ORDER TO HAVE WARRANTEES IN FORCE. ONE SHOULD REQUIRE THAT ACCEPTANCE OF THE EQUIPMENT NOT START UNTIL THE ENTIRE SYSTEM HAS BEEN INSTALLED. ONCE ONE HAS INDICATED ACCEPTANCE OF PART OF A SYSTEM A PERIPHERAL INSTALLED LATER MAY REVEAL A DEFECT IN THE DEVICE WHICH DOES NOT VIOLATE THE DEVICE SPECIFICATIONS. SUCH DESIGN DEFECTS ARE COMMON. ACCEPTANCE SHOULD BE CARRIED OUT WITH CARE, IN A CONSCIOUS ATTEMPT TO DISPLAY WEAKNESSES IN ANY PARTS. THIS WILL CONSUME MUCH TIME FOR THE USER, BUT AVOID GREATER TROUBLE LATER IN THE LIFE OF THE EQUIPMENT. ACCEPTANCE CRITERIA SHOULD BE AGREED ON IN ADVANCE AND PROVEN TO HAVE BEEN MET BY A WRITTEN RECORD MAINTAINED BY THE USER, RATHER THAN BY THE VENDOR. PARTIAL ACCEPTANCE, OR CONDITIONAL ACCEPTANCE, OR ANYTHING ELSE LESS THAN FULL ACCEPTANCE IS USUALLY A MISTAKE. ONE IS SOMETIMES FORCED INTO SUCH A POSITION, BUT THEN ONE IS ADVISED TO HAVE THE SITUTATION SPELLED OUT IN PAINFUL DETAIL IN WRITING, WITH HARSH PENALTIES FOR FAILURE TO MEET ANY DEFERRED DEADLINES.

III. CRYSNET TERMINAL OPERATIONS

1. TERMINAL OPERATIONS OVERVIEW

A CRYSNET TERMINAL IS RUN "HANDS-ON" BY ONE PERSON AT A TIME. ONE FUNCTIONS AS ONE'S OWN COMPUTER OPERATOR. ONE MUST KNOW HOW TO START THE MACHINE, INCLUDING EACH OF THE PERIPHERAL DEVICES ONE WILL USE. ONE MUST KNOW HOW TO PROPERLY STOP EVERYTHING ONE HAS STARTED. ONE MUST KNOW HOW TO RUN THE PROGRAMS ONE NEEDS, HOW TO TERMINATE THEM, AND HOW TO DECIDE IF TROUBLE HAS BEEN ENCOUNTERED. IF TROUBLE HAS BEEN ENCOUNTERED, ONE MUST BE ABLE TO DETERMINE IF THE FAULT IS IN ONE'S USE, EQUIPMENT FAILURE, HARDWARE FAILURE, OR SOMETHING ONE DOES NOT UNDERSTAND. EITHER ONE MUST KNOW HOW TO CORRECT TROUBLE, OR HOW TO REPORT TROUBLE TO SOMEONE ELSE WHO CAN DO SO. SOME KEY USER MUST KNOW HOW TO CREATE, UPDATE, AND BACK UP OPERATING SYSTEMS, MAINTAIN LOGS AND MANUALS, ORDER SUPPLIES, CLEAN EQUIPMENT, REPLACE PAPER PRODUCTS, RUN DIAGNOSTICS AND CALL IN SERVICE PEOPLE. THIS KEY USER MUST ALSO ENSURE AN EQUITABLE DISTRIBUTION OF ACCESS TO THE MACHINE, AND MONITOR THE CONTRACTS AND FUNDS NECESSARY TO THE CONTINUED EXISTENCE OF THE FACILITY.

THIS DISTINCTION BETWEEN USERS AND THE KEY USER IS SOMEWHAT ARTIFICIAL. IN SOME SHOPS, THE FUNCTION OF KEY USER WILL DEVOLVE ON ONE UNFORTUNATE SOUL, WHO DOES EVERYTHING FROM CLEANING UP TO CHASING VENDORS, WHILE IN OTHERS THE FUNCTIONS WILL BE DISTRIBUTED AMONG ALL USERS. WE WILL MAINTAIN THE PRETENCE THAT THE KEY USER IS A DISTINCT PERSON, AND SAVE THE DESCRIPTION OF HIS RESPONSIBILITIES TO THE END OF THIS CHAPTER.

THE BASIC REFERENCE FOR THE OPERATION OF THIS TERMINAL IS "THE DOS/BATCH HANDBOOK", DEC PUBLICATION NUMBER DEC-11-ODBHA-A-D. THIS BOOK CONTAINS INFORMATION ON ALL THE MAJOR SYSTEM UTILITY PROGRAMS. IT ALSO PROVIDES COMPLETE VENDOR DOCUMENTATION FOR MOST USERS. SOME CIRCUMSTANCES WILL REQUIRE REFERENCE TO "THE DOS/BATCH SYSTEM MANAGER'S GUIDE", DEC PUBLICATION NUMBER DEC-11-OSMGA-A-D. NORMALLY ONLY THE KEY USER WILL HAVE NEED OF THAT MANUAL. A USER WITH INTEREST IN THE INTERNALS OF THE SYSTEM SHOULD READ "THE DOS/BATCH SOFTWARE SUPPORT MANUAL", DEC PUBLICATION NUMBER DEC-11-OSSMA-A-D, AND "THE DOS/BATCH DEVICE DRIVER PACKAGE PROGRAMMER'S MANUAL", DEC PUBLICATION NUMBER DEC-11-ODDPB-A-D, AS WELL AS THE "PDP11 PERIPHERALS HANDBOOK" (ORDER BY TITLE FROM DEC). A PROGRAMMER WISHING TO PROGRAM FOR THE DISPLAY SHOULD READ "FORTRAN DRAWING PACKAGE REFERENCE MANUAL (FDP)", VECTOR GENERAL DWG. NUMBER 910823.

2. GETTING ON THE TERMINAL

IN ORDER TO GET ON THE TERMINAL, ONE MUST FIRST ARRANGE THE RIGHT TO GET ON, ARRANGE A TIME TO GET ON, AND THEN ACTUALLY GET ON. ONE MUST KNOW HOW TO START UP THE DEVICES NEEDED, AND INFORM THE SYSTEM OF WHAT ONE WISHES TO DO.

2.1. ARRANGING ACCESS

ACCESS TO THE TERMINAL IS CONTROLLED BY THE KEY USER. ONE MUST ARRANGE WITH HIM TO BE ENTERED AS A VALID USER IN HIS RECORDS, AND BE GIVEN A USER IDENTIFICATION CODE. THIS "UIC" IS A PAIR OF NUMBERS USED TO SEPARATE ONE'S FILES ON ALL MEDIA FROM THOSE BELONGING TO OTHERS. USE OF THE WRONG UIC CAN CAUSE GREAT CONFUSION AND POSSIBLE LOSS OF DATA ONE MAY WISH TO RETAIN. SOME USERS WILL BE RUNNING ONLY A LIMITED SET OF APPLICATIONS PROGRAMS, AND WILL NOT REQUIRE THE ABILITY TO RETAIN FILES. SUCH A USER MAY BE GIVEN A UIC THE SAME AS THAT USED BY OTHER USERS IN A SIMILAR SITUATION. SUCH A USER MUST BE AWARE OF THIS AND RETURN TO THE KEY USER FOR A NEW UIC, IF HIS NEEDS CHANGE, REQUIRING THAT HE HAVE MORE GENERAL ACCESS TO THE SYSTEM.

2.2. GETTING TIME

ONCE ONE IS AUTHORIZED TO USE THE TERMINAL, ONE MUST STILL MAKE PROPER ARRANGEMENTS FOR EACH SESSION ON THE TERMINAL. NEAR THE TERMINAL, ONE CAN FIND TWO BOOKS. ONE IS A LOG BOOK, INDICATING CURRENT USE OF THE TERMINAL, AND ONE IS A SIGN-UP BOOK INDICATING FUTURE REQUESTS FOR TIME. IF NO-ONE IS SIGNED IN THE LOG BOOK, AND NO-ONE HAS REQUESTED THE IMMEDIATELY FOLLOWING PERIOD, JUST TAKE THE MACHINE. OTHERWISE, ONE MUST FIND A SUITABLE FREE PERIOD IN THE SIGN-UP BOOK AND ENTER A REQUEST. THE KEY USER WILL ESTABLISH THE MAXIMUM PERMISSIBLE SINGLE TIME REQUEST AND NUMBER OF REQUESTS FOR EACH USER. IT IS USUALLY IMPROPER TO SIGN FOR MORE THAN ONE FUTURE SLOT AT A TIME, AND FOR MORE THAN ONE HOUR AT A TIME. IF A USER IS ON THE TERMINAL AT THE TIME OF ENTERING A REQUEST, IT IS CONSIDERED COURTEOUS TO ALLOW THE USER WHO IS ON AT LEAST HALF AN HOUR TO FINISH HIS OR HER WORK, EVEN IF THAT USER SIMPLY TOOK THE MACHINE WITHOUT ENTERING A REQUEST. HOWEVER, A USER WHO TAKES THE MACHINE AFTER REQUESTS HAVE BEEN PLACED IN THE SIGN-UP BOOK IS RESPONSIBLE FOR PACING HIS OR HER WORK TO BE OFF THE TERMINAL AT THE PROPER TIME.

2.3. TURNING ON THE TERMINAL

IF ALL EQUIPMENT IS PROPERLY TURNED ON AT THE START OF THE SESSION, SKIP THIS SECTION. THE MESSAGE "A002" USUALLY MEANS THAT SOMETHING HAS NOT BEEN TURNED ON. IN THAT CASE, READ THIS SECTION.

THIS SECTION ASSUMES THE STANDARD TERMINAL CONFIGURATION. IT WILL HAVE TO BE MODIFIED TO MEET ACTUAL LOCAL CONDITIONS.

THE PRECISE EQUIPMENT WHICH MUST BE TURNED ON VARIES WITH THE CONDITION IN WHICH THE TERMINAL HAS BEEN LEFT BY THE LAST USER. NORMALLY, ELECTRONIC EQUIPMENT SHOULD BE LEFT ON AT ALL TIMES. THIS GREATLY INCREASES THE LIFE AND STABILITY OF COMPONENTS. HOWEVER, SOME PARTICULARLY NOISY DEVICES MAY HAVE BEEN SWITCHED OFF, OR LOCAL REGULATIONS MAY EVEN HAVE REQUIRED A COMPLETE POWER-DOWN OVERNIGHT. IN ORDER TO UNDERSTAND THE METHODS FOR TURNING ON EQUIPMENT, ONE MUST REALIZE THAT FOR EACH DEVICE THERE ARE USUALLY CONTROL SYSTEMS NOT NECESSARILY CONTROLLED BY SWITCHES ON THE DEVICE. IN THAT CASE, ONE MUST BE CAREFUL TO TURN ON THE CONTROL ELECTRONICS BEFORE TURNING ON THE DEVICE. SINCE THE COMPUTER ITSELF IS THE ULTIMATE CONTROL DEVICE, IT SHOULD BE TURNED ON FIRST. SINCE THE DISPLAY HAS PARTICULARLY BAD POWER-UP/POWER-DOWN CHARACTERISTICS, IT SHOULD BE TURNED ON NEXT, AND LEFT ON. THEN ONE SHOULD TURN ON EACH OF THE PERIPHERALS ONE THINKS ONE MIGHT NEED IN THE SESSION. THE POWER SWITCH LOCATIONS FOR A TYPICAL SYSTEM ARE AS FOLLOWS:

COMPUTER - THERE IS A REMOVABLE KEY ON THE LEFT OF THE FRONT PANEL OF THE COMPUTER. IT SHOULD ALWAYS BE THERE. ROTATION TO THE EXTREME COUNTER-CLOCKWISE POSITION TURNS OFF THE COMPUTER AND MOST ASSOCIATED PERIPHERALS MOUNTED WITHIN THE COMPUTER CABINETS. THE NEXT CLOCKWISE POSITION PROVIDES POWER TO THE COMPUTER AND THOSE PERIPHERALS. THE FINAL CLOCKWISE POSITION SHOULD NOT BE USED, AS IT DISABLES THE CONSOLE SWITCHES ONE NEEDS TO START THE SYSTEM. IT IS BEST TO BE CERTAIN THE "HALT-ENABLE" SWITCH ON THE RIGHT OF THE FRONT PANEL IS IN THE HALT POSITION BEFORE APPLYING POWER.

DISPLAY - THERE IS A POWER SWITCH AT FLOOR LEVEL ON THE REAR OF THE DISPLAY, SOMEWHAT TO THE LEFT AS ONE FACES IT FROM BEHIND. DOWN IS OFF, UP IS ON. DO NOT USE A FOOT TO WORK THIS SWITCH. USE A HAND, EVEN IF ONE MUST GET ON ONE'S KNEES TO DO SO.

DISC DRIVE - THERE IS NO SEPARATE POWER SWITCH ON MOST MODELS OF THE DISC DRIVE, BUT THERE IS A "RUN-LOAD" SWITCH WHICH CONTROLS MOTOR POWER. THIS SWITCH SHOULD BE IN THE LOAD POSITION WELL BEFORE ANY POWER-DOWN OF THE COMPUTER, TO ALLOW TIME FOR THE HEADS TO RETRACT. WITH A DISC IN, THIS SWITCH SHOULD BE IN THE RUN POSITION AT ALL TIMES. ONE SHOULD VERIFY THAT THE DISC THAT IS IN, MATCHES A SIGN ON THE DRIVE INDICATING WHICH DISC SHOULD BE MOUNTED.

OPERATOR CONSOLE DEVICE - THERE ARE MANY ALTERNATE OPERATOR CONSOLE DEVICES - SOME WITH A KEYBOARD AND HARD-COPY PRINTER, AND SOME WITH A KEYBOARD AND DISPLAY. USUALLY POWER WILL BE CONTROLLED BY THE POWER SWITCH ON THE COMPUTER. HOWEVER, A

SEPARATE POWER SWITCH ON THE CONSOLE MAY WELL HAVE BEEN USED BY THE PERSON SHUTTING DOWN. ON AN ASR-33, THE POWER SWITCH IS A ROTARY SWITCH ON THE FRONT RIGHT OF THE DEVICE, WHICH SHOULD BE PLACED IN THE "LINE" POSITION TO BOTH APPLY POWER AND CONNECT TO THE COMPUTER.

MAGNETIC TAPE DRIVE - IT IS VERY UNDESIRABLE TO TURN THE POWER OFF FOR THIS DEVICE. THERE IS AN "ON-OFF" SWITCH ON THE LOWER LEFT PANEL (UPPER LEFT SWITCH) BUT THIS IS BEST TAPED IN THE ON POSITION. ONE SHOULD CHECK THAT THE "UNIT" SWITCH IS SET TO A NUMBER MATCHING A LABEL ON THE DRIVE.

PRINTER/PLOTTER - THERE IS A POWER SWITCH ON THE UPPER RIGHT OF THE TOP OF THE PRINTER.

CARD READER - THERE IS A POWER SWITCH AT THE TOP REAR OF THE READER, ON THE LEFT FACING IT FROM THE REAR, ON THE RIGHT REACHING OVER FROM THE FRONT AS MOST PEOPLE DO.

ONE SHOULD BE AWARE THAT SOME OF THE POWER SWITCHES DO NOT TOTALLY DISCONNECT ALL WIRES WITHIN A DEVICE FROM THE POWER LINES. IF ONE MUST ENTER EQUIPMENT WITHOUT CERTAIN KNOWLEDGE OF ITS WORKINGS, IT IS BEST TO DISCONNECT POWER BY THROWING ALL BREAKERS AND TESTING WITH A METER. ONE SHOULD ALSO BE AWARE THAT WHEN POWER IS APPLIED TO THE DEVICES OF THIS TERMINAL, THEY DO NOT MAKE NOISES THAT ONE MIGHT INTERPRET AS EQUIPMENT DESTROYING ITSELF. SHOULD SUCH NOISES BE HEARD, DISCONNECT POWER AT ONCE.

2.4. STARTING A SESSION

THE VERY FIRST ACTION TO BE TAKEN AT THE START OF A SESSION IS TO SIGN THE LOG BOOK. THIS MUST BE DONE FOR TWO REASONS. FIRST, BY SO DOING, ONCE IS FORCED TO LOOK AT THE LOG BOOK AND SEE IF THE PRIOR USER ACTUALLY SIGNED OFF THE MACHINE. IF THAT USER DID NOT SIGN OFF, PERHAPS HE IS NOT DONE, AND SHOULD BE ASKED. SECOND, THE LOG BOOK IS THE ONLY RELIABLE RECORD OF PROBLEMS WITH THE TERMINAL. BY KNOWING WHO WAS USING THE MACHINE AT PARTICULAR TIMES IT IS OFTEN EASIER TO DEFINE PROBLEMS PRECISELY.

ONCE ALL EQUIPMENT IS ON, ONE MUST GET THE RIGHT PROGRAMS RUNNING. PROGRAMS DO NOT RESIDE IN THE COMPUTER ITSELF, EXCEPT WHEN THEY ARE ACTUALLY RUNNING. ALL PROGRAMS MUST COME EITHER FROM TAPE OR DISC. MOST PROGRAMS RUN BY USERS ARE CONTROLLED BY A COMMON PROGRAM CALLED THE "DOS/BATCH OPERATING SYSTEM". SOME DIAGNOSTICS RUN OUTSIDE THIS ENVIRONMENT. FOR THEM, SEE THE SECTION ON "RUNNING MAINTENANCE PROGRAMS". FOR OTHER PROGRAMS, ONE MUST FIRST LOAD THE OPERATING SYSTEM. IF THE LAST USER LEFT THE MACHINE IN ITS NORMAL CONDITION, THERE IS LITTLE TO DO, SINCE A COPY OF THE MONITOR SHOULD STILL BE IN

EXECUTION. IF THERE HAS BEEN A POWER FAILURE, HOWEVER, OR THE PRIOR USER RAN FROM A DIFFERENT DISC, ONE MUST "REBOOT" THE SYSTEM. TO DO SO, SEE "BOOTSTRAP PROCEDURE", BELOW.

WHEN THE MONITOR IS WAITING FOR A COMMAND TO RUN A PROGRAM, IT WILL HAVE PRINTED

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$*
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THE COMPUTER AND MOST PROGRAMS EXPECT COMMANDS OR DATA FROM THE KEYBOARD TYPED AS LINES OF CHARACTERS TERMINATED BY A CARRIAGE RETURN ("NEW LINE" ON SOME CONSOLES). UNTIL THAT TERMINATING CHARACTER IS TYPED, THE USER IS FREE TO CHANGE HIS MIND ABOUT THE CONTENTS OF THE LINE. ONE MAY ERASE A SINGLE CHARACTER BY TYPING "RUBOUT" ("DEL" ON SOME MACHINES). THE TERMINAL WILL RESPOND BY TYPING THE CHARACTERS ERASED, IN THE ORDER ERASED, BETWEEN REVERSE SLASHES. AN ENTIRE LINE MAY BE ERASED BY TYPING "CONTROL-U" (HOLD DOWN THE "CONTROL" KEY AND WHILE STILL HOLDING IT DEPRESS "U").

THE FIRST COMMAND SEQUENCE TO BE GIVEN BEFORE RUNNING A PROGRAM IS

```
FI
LO NNN,NNN
```

WHERE THE FIRST COMMAND ("FI" FOR FINISH) CAUSES THE MONITOR TO BE REFRESHED FROM THE DISC, AND THE SECOND COMMAND ("LO" FOR LOGIN) IDENTIFIES THE USER TO THE SYSTEM. THE NUMBER IN THE LOGIN COMMAND "NNN,NNN", IS THE ASSIGNED UIC, E.G. "100,100". THERE IS NO PUNCTUATION OTHER THAN A BLANK BETWEEN THE "LO" AND THE DIGITS OF THE UIC, WHICH ARE SEPARATED INTO A GROUP NUMBER AND USER NUMBER BY A COMMA. THE FIRST TIME A USER LOGS IN, HE MUST ALSO

```
RU PIP
/EN
(CONTROL-D)
```

IN ORDER TO CREATE THE TABLES ON DISC NEEDED TO WRITE FILES. THIS IS NORMALLY DONE BY THE KEY USER.

ONE CAN NOW RUN A PROGRAM BY USE OF THE "RUN" COMMAND. IF THE PROGRAM IS MAINTAINED ON THE DISC AS PART OF THE LIBRARY UNDER THE UIC [1,1], AND HAS THE NAME "PRONAM", THEN ONE MAY RUN THE PROGRAM SIMPLY BY

```
RU "PRONAM"
```

FOR EXAMPLE TO RUN THE PROGRAM PRJCTN, ONE MIGHT TYPE

```
RU PRJCTN
```

WHICH WOULD START THE PROGRAM PRJCTN INTO EXECUTION. HOWEVER, NOT ALL PROGRAMS ARE MAINTAINED UNDER "1,1", SO ONE MUST BE AWARE OF THE PROCEDURES FOR RUNNING PROGRAMS RESIDING ELSEWHERE.

IF THE PROGRAM RESIDES AMONG THE FILES ON DISC OF A PARTICULAR USER WITH UIC "NNN,NNN", AND NAME "PRONAM", THEN ONE WOULD RUN THAT PROGRAM

BY

```
RU "PRONAM"["NNN,NNN"]
```

E.G.

```
RU PRJCTN[100,100]
```

IF THE PROGRAM RESIDES ON A MAGNETIC TAPE, ONE MUST MOUNT THAT TAPE, PUT THE UNIT ON LINE AND TYPE THE COMMAND

```
RU MT"UNIT":"PRONAM".LDA["NNN,NNN"]
```

WHERE "UNIT" IS THE UNIT NUMBER OF THE TAPE DRIVE, "PRONAM" IS THE PROGRAM NAME, AND "NNN,NNN" IS THE UIC UNDER WHICH THE PROGRAM WAS WRITTEN ON TAPE. FOR EXAMPLE

```
RU MT0:S4010.LDA[20,20]
```

BE WARNED THAT OVERLAYED PROGRAMS CANNOT BE RUN FROM TAPE.

ONCE A PROGRAM HAS BEEN STARTED, IT IS IN CONTROL, AND THE OPERATING INSTRUCTIONS FOR THAT PARTICULAR PROGRAM MUST BE FOLLOWED.

3. GETTING OFF THE TERMINAL

WHEN ONE IS DONE RUNNING WHATEVER PROGRAMS ONE WISHES TO USE, ONE IS RESPONSIBLE FOR CLEANING ANY UNNECESSARY FILES FROM THE DISC, RETURNING ANY TAPES OR CARD DECKS TO THEIR STORAGE AREAS, TURNING OFF THOSE FEW DEVICES WHICH SHOULD NORMALLY BE SHUT DOWN (THE CARD READER AND PRINTER IN MOST INSTALLATIONS), AND SIGNING OUT FROM THE LOG BOOK. NATURALLY, ONE SHOULD POLICE THE AREA FOR ANY BOOKS, PAPERS OR OTHER PERSONAL EFFECTS LEFT IN COMMON AREAS.

3.1. ENDING A SESSION

TO TERMINATE A SESSION, ONE MUST STOP ANY RUNNING PROGRAM, DELETE ANY FILES WHICH ARE NOT NEEDED, AND EXECUTE THE "FI" (FINISH) COMMAND TO ALLOW THE NEXT USER TO LOGIN.

TO TERMINATE A PROGRAM FOR WHICH NO OTHER TERMINATION IS PROVIDED, ONE MAY USE THE COMMAND "KILL". TO MAKE THE MONITOR PAY ATTENTION TO THIS COMMAND, ONE MAY FIRST HAVE TO TYPE "CONTROL-C". IN THAT CASE, THE COMMAND "WAIT" SHOULD BE TYPED BEFORE "KILL" TO ALLOW AS MUCH INPUT/OUTPUT TO STOP AS POSSIBLE. BE WARNED THAT TERMINATING A PROGRAM THIS WAY OFTEN CAUSES FILES WHICH WERE IN THE PROCESS OF BEING WRITTEN TO BE IMPROPERLY TERMINATED. SUCH FILES MUST BE DELETED BEFORE LEAVING THE MACHINE TO ANOTHER USER. THIS IS DONE BY RUNNING PIP AND USING THE "/DE" SWITCH. FOR EXAMPLE

```
RU PIP
```

```
EDITOR.TMP/DE
```

A LIST OF ALL CURRENT FILES MAY BE FOUND BY USE OF THE "/DI" SWITCH. FOR EXAMPLE

```
RU PIP
/DI
```

WHICH WILL LIST THE NAMES OF FILES ON THE CONSOLE. WHILE

```
RU PIP
VLT</DI
```

WILL LIST THE NAMES OF ALL FILES ON THE PRINTER. PLEASE REMEMBER THAT PIP IS ITSELF A PROGRAM, AND MUST BE TERMINATED BY "CONTROL-C" AND "KILL".

THE SESSION ITSELF IS ENDED BY TYPING THE COMMAND "FI" (FINISH). ONE SHOULD THEN SIGN OUT OF THE LOG BOOK, NOTING ANY UNUSUAL EVENTS WHICH WERE NOT YET RECORDED.

IF ONE IS UNABLE TO TERMINATE A SESSION PROPERLY, ONE SHOULD NOT JUST WALK AWAY. IF AT ALL POSSIBLE, GET HELP. IF NOT, PLEASE LEAVE A LARGE SIGN TO THAT EFFECT TAPED TO THE MACHINE. THIS WILL GIVE THE NEXT USER A CHANCE TO STAIGHTEN THINGS OUT BEFORE HE WORKS WITH A CLOBBERED DISC AND LOSES A SESSION.

3.2. TURNING OFF EQUIPMENT

EQUIPMENT IS POWERED DOWN BY FIRST TURNING OFF THE DEVICES ELECTRICALLY FURTHEST FROM THE COMPUTER AND TURNING OFF THE COMPUTER LAST. EXCEPT IN AN EMERGENCY, NO USER SHOULD TAKE IT UPON HIMSELF TO TURN OFF ANY EQUIPMENT WHEN HE HAS NOT BEEN TOLD EXPLICITLY TO TURN OFF. THE ONLY DEVICES WHICH SHOULD BE TURNED OFF IN THE NORMAL COURSE OF ENDING A SESSION ARE THE CARD READER AND PRINTER/PLOTTER. ALL OTHER DEVICES SHOULD BE LEFT ON.

4. FILE SPECIFICATIONS

DOS/BATCH MAKES EXTENSIVE USE OF "FILE SPECIFICATIONS" TO IDENTIFY WHICH DEVICES AND PORTIONS OF DEVICES ARE TO BE USED BY A PROGRAM FOR ITS DATA. A FILE IS SPECIFIED BY A CHARACTER STRING SUCH AS:

"DEV""UNIT":"FILNAM"."EXT"["NNN,NNN"]

WHERE "DEV" IDENTIFIES THE DEVICE, "UNIT" IDENTIFIES THE UNIT IN CASE OF A MULTIPLE UNIT DEVICE, "FILNAM" IDENTIFIES WHICH ONE OF MANY FILES ON A "FILE-STRUCTURED" DEVICE IS BEING USED, "EXT" PROVIDES AN OPTIONAL EXTENSION TO THE FILENAME TO FURTHER SEPARATE FILES, AND "NNN,NNN" IS THE UIC FOR THE USER WHO MADE THE FILE.

A DEVICE NAME AND UNIT NUMBER ARE ALWAYS TERMINATED BY A COLON. IF THE COLON IS LEFT OUT, THE DEVICE NAME LOOKS LIKE A FILENAME TO THE SYSTEM, INSTEAD OF LIKE A DEVICE NAME. THE ONLY DEVICES WHICH WILL HAVE UNIT NUMBERS ON AN ORDINARY CRYSNET TERMINAL ARE THE MAGNETIC TAPE DRIVE AND THE DISC. THE DEVICES ARE:

CR:	CARD READER
KB:	CONSOLE KEYBOARD AND PRINTER (OR DISPLAY)
PT:	CONSOLE PAPER TAPE READER/PUNCH (NOT ON ALL)
PR:	HIGH SPEED PAPER TAPE READER (NOT ON ALL TERMINALS)
PP:	HIGH SPEED PAPER TAPE PUNCH (NOT ON ALL TERMINALS)
VL:	VERSATEC LINE PRINTER (NO FORTRAN CARRIAGE CONTROL)
LP:	" " " " " " (WITH FORTRAN CARRIAGE CONTROL)
VP:	VERSATEC PLOTTER
MT0:	MAGNETIC TAPE UNIT 0 (USUALLY NINE TRACK)
MT1:	MAGNETIC TAPE UNIT 1 (USUALLY SEVEN TRACK)
DK0:	DISC UNIT 0 (USUALLY HAS SYSTEM ON IT)
DK1:	DISC UNIT 1 (NOT ON ALL TERMINALS)
SY:	SYSTEM DEVICE (DK0:) A COMMON DEFAULT
NU:	NULL DEVICE (INFINITE SINK, SOURCE OF EOF'S)

"FILNAM" MAY BE ANY SIX LETTERS OR DIGITS TO IDENTIFY A FILE ON DISC OR TAPE. "EXT" MAY BE ANY THREE LETTERS OR DIGITS TO EXTEND THE FILENAME. ".OBJ" IS USUALLY USED FOR BINARY CODE PRODUCED BY THE COMPILER, ".LDA" IS USUALLY USED FOR BINARY CODE PRODUCED BY THE LINKER. IT IS GOOD PROGRAMMING PRACTICE TO USE ".FTN" FOR FORTRAN SOURCE CODE AND ".MAC" FOR MACRO SOURCE CODE.

IN MANY SYSTEM MESSAGES, ESPECIALLY A002 (DEVICE NOT READY) AND F012 (FILE NOT FOUND), THE ACTUAL DEVICE NAME APPEARS IN A CODED FORM CALLED "RADIX-50". THE CODES FOR THE DEVICES ON THE TERMINAL ARE

012620 FOR CR:
015270 FOR DK:
046600 FOR LP:
052140 FOR MT:
063200 FOR PP:
063320 FOR PR:
015270 FOR SY:
105540 FOR VL:
106000 FOR VP:

FOR EXAMPLE IF A PROGRAM STOPS WITH

A002 012620

ONE HAS A PROBLEM WITH THE CARD READER. ONE SHOULD CORRECT THE PROBLEM, READY THE READER, AND TYPE "CO" (CONTINUE) TO GET THE PROGRAM TO CONTINUE PROCESSING. IF ONE CANNOT CORRECT THE PROBLEM, ONE SHOULD TYPE THE COMMAND "KI" (KILL). FOR AN F012, "KI" IS THE ONLY CORRECT RESPONSE.

5. BOOTSTRAP PROCEEDURES

THIS SECTION IS NORMALLY FOR USE BY THE KEY USER. FOR DETAILED INFORMATION ON BOOTSTRAP PROCEDURES, ONE SHOULD REFER TO APPENDIX G OF THE "DOS/BATCH HANDBOOK".

THE CRYSNET TERMINAL IS USUALLY RESTARTED FROM DISC. THE EXACT PROCEDURE DEPENDS UPON WHICH BOOTSTRAP DEVICE, IF ANY, EXISTS IN THE MACHINE. THERE ARE THREE MAJOR POSSIBILITIES: THE MR11-DB, THE BM873-YA, OR BM873-YB. ALL THREE HAVE SIMILAR OPERATING INSTRUCTIONS, EXCEPT THAT THE "START ADDRESS" IS DIFFERENT. A LABEL SHOULD BE PASTED DIRECTLY ABOVE THE CONSOLE SWITCH REGISTER WITH THE CORRECT ADDRESS.

ALL NEEDED EQUIPMENT SHOULD BE POWERED UP. THE CORRECT SYSTEM DISC SHOULD BE IN THE DRIVE AND "ON LINE". THERE IS A SET OF 18 SWITCHES ON THE FRONT OF THE COMPUTER WITH NUMBERS 0 THROUGH 17. THESE ARE CALLED THE "SWITCH REGISTER". TO THE RIGHT OF THESE SWITCHES ARE "LOAD ADDRESS", "HALT/ENABLE", AND START" SWITCHES NEEDED TO BOOTSTRAP THE COMPUTER.

1. MOVE THE "HALT/ENABLE" SWITCH TO "HALT". MOMENTARILY DEPRESS "START" TO CLEAR ANY HANGS.

2. SET THE CORRECT ADDRESS IN THE SWITCH REGISTER:

773110 FOR MR11
773010 FOR BM873-YA
773030 FOR BM873-YB

THUS FOR THE MR11 ONE WOULD RAISE SWITCHES 17, 16, 15, 14, 13, 12, 10, 9, 6, AND 3 AND LOWER THE OTHER NUMBERED SWITCHES. THE BM873-YA WOULD BE THE SAME, EXCEPT THAT SWITCH 6 WOULD BE DOWN, WHILE THE BM873-YB WOULD HAVE SWITCH 6 DOWN AND SWITCH 4 RAISED.

3. MOVE "HALT/ENABLE" TO "ENABLE".

4. DEPRESS "START" AGAIN.

AT THIS POINT THE COMPUTER SHOULD ASK FOR THE DATE AND TIME. IT IS POSSIBLE ON AN ADDS TERMINAL TO GET A BLACK LINE INSTEAD. IN THAT CASE, TYPE "NEW LINE" AND THE SITUATION SHOULD CLEAR ITSELF. ON SOME OTHER

MODELS OF ADDS TERMINALS, ONE IS OBLIGED TO TYPE "INSERT" BEFORE "NEW LINE".

5. ENTER DATE AND TIME. TYPE THE DATE AS TWO DIGITS FOR THE DAY, A HYPHEN, THE FIRST THREE CHARACTERS OF THE MONTH, A HYPHEN, AND THE LAST TWO DIGITS OF THE YEAR. FOLLOW WITH A "CARRIAGE RETURN" ("NEW LINE" ON SOME TERMINALS). THE COMPUTER WILL THEN ASK FOR THE TIME. REPLY WITH THE TIME ON THE BASIS OF A 24-HOUR CLOCK, WITH A COLON BETWEEN THE HOURS AND MINUTES, AS IN "13:45". FOLLOW WITH A "CARRIAGE RETURN" ("NEW LINE" ON SOME TERMINALS).

6. ANSWER THE DIALOG QUESTIONS. THE COMPUTER WILL ASK IF YOU WISH A DIALOG. THE ANSWER SHOULD BE "Y" FOLLOWED BY A "CARRIAGE RETURN". IT WILL THEN ASK A SERIES OF QUESTIONS ABOUT VARIOUS DEVICES. EXCEPT FOR THE QUESTION "CHANGE CARD READER DEFAULTS", THE ANSWER SHOULD BE "N" FOLLOWED BY A "CARRIAGE RETURN". THE ANSWER FOR THE CARD READER SHOULD BE "Y" FOLLOWED BY A "CARRIAGE RETURN". THE ANSWER TO "BINARY SUPPORT" SHOULD NORMALLY BE "N", BUT IF ONE WISHED TO RUN DIAGNOSTICS FROM CARDS, IT WOULD HAVE TO BE "Y". THIS WOULD REQUIRE THE USE OF THE "/FA" SWITCH WHEN RUNNING PIP TO COPY CARD DECKS IN AS SOURCE CODE. THE CORRECT CARD CODE DEFAULT DEPENDS ON THE INSTALLATION. IF A CDC CENTRAL SITE IS BEING USED, "CDC 026" MAY DESERVE A "Y". (THIS IS TRUE AT BNL).

THE SYSTEM SHOULD NOW BE ALIVE WITH A "$*" ON THE CONSOLE. IT SOMETIMES HAPPENS THAT A BOOTSTRAP WILL HANG PART WAY THROUGH, OR JUST AT THIS POINT. THIS USUALLY IS DUE EITHER TO A DIRTY DISC OR TO A DISC AT AN IMPROPER TEMPERATURE. IN EITHER CASE, ONE CAN OFTEN GET ON THE AIR BY JUST TRYING THE BOOTSTRAP PROCEDURE AGAIN. IF THIS STILL DOESN'T WORK, TRY ANOTHER DISC. IF IT STILL FAILS, REQUEST SERVICE.

6. MOUNTING MEDIA

IN RUNNING THE TERMINAL, IT IS OFTEN NECESSARY TO MOUNT MAGNETIC TAPES, CARD DECKS, DISC PACKS, AND PRINTER PAPER. THE GENERAL RULE IS NEVER FORCE ANYTHING THAT SEEMS STUCK. IF IN DOUBT ABOUT INSTRUCTIONS FOR HANDLING A DEVICE, ONE SHOULD ASK FOR HELP. IT IS QUITE POSSIBLE TO TOTALLY DESTROY A DISC DRIVE OR TAPE DRIVE BY CARELESSNESS. THE FIRST TIME ONE HANDLES ANY EQUIPMENT ON THE TERMINAL IT SHOULD BE UNDER THE SUPERVISION OF AN EXPERIENCED INDIVIDUAL.

6.1. MOUNTING TAPE REELS

MAGNETIC TAPES CONSIST OF HALF-INCH WIDE MYLAR COATED WITH IRON OXIDE, WOUND BETWEEN TWO PLASTIC FLANGES ON A HUB. ONE MUST NEVER EXERT PRESSURE WHICH WOULD PRESS THE FLANGES TOGETHER. AS MUCH AS POSSIBLE, THE TAPE SHOULD BE HANDLED AT THE HUB. SINCE MAGNETIC TAPES ARE VERY SENSITIVE TO DIRT, CARE MUST BE TAKEN NOT TO HANDLE THE OXIDE OF THE TAPE. NATURALLY, ONE MUST NOT SMOKE NEAR MAGNETIC TAPES (NOR NEAR ANY COMPUTER EQUIPMENT).

IN ORDER TO MOUNT A MAGNETIC TAPE, ONE STARTS WITH THE TAPE IN ITS CANNISTER OR TAPE SEAL, AND THE TAPE DRIVE FREE. HANDLING THE TAPE BY THE HUB, REMOVE IT FROM THE CANNISTER AND CLOSE THE CANNISTER. THEN OPEN THE TAPE DRIVE DOOR (THERE IS A LATCH ON THE LEFT AT ABOUT SHOULDER LEVEL). PLACE THE TAPE FIRMLY ON THE LOWER HUB WITHOUT PRESSING ON THE TAPE FLANGES. TURN THE HUB LOCK CLOCKWISE UNTIL THE TAPE IS FIRMLY HELD. PUT THE "BRAKE RELEASE/LOAD" SWITCH IN THE BRAKE RELEASE POSITION. THE LOWER HUB SHOULD NOW TURN FREELY. THREAD THE TAPE UP OVER THE LOWER TAPE GUIDE, THROUGH THE SLOT IN FRONT OF THE HEAD, OVER THE RUBBER CAPSTAN, AND THEN ALL THE WAY TO THE LEFT TO COME AROUND THE UPPER TAPE GUIDE, AND THEN BACK TO THE RIGHT TO WIND AROUND THE TAKE-UP REEL. WIND ABOUT FIVE TURNS OF TAPE ONTO THE TAKE-UP REEL AND THEN MOVE THE "BRAKE RELEASE/LOAD" SWITCH TO LOAD. ONCE THE TAPE HAS LOADED INTO THE VACUUM COLUMNS, PUT THE "ON LINE/OFF LINE" SWITCH TO "OFF LINE" AND THE "FORWARD/REWIND/REVERSE" SWITCH TO "FORWARD". PUT THE "STOP/START" SWITCH FIRST TO "STOP" AND THEN TO "START". THE TAPE SHOULD NOW MOVE FORWARD TO LOAD POINT. IF IT SEEMS TO RUN AWAY, PUT THE "STOP/START" SWITCH TO "STOP", THE "FORWARD/REWIND/REVERSE" SWITCH TO "REWIND" AND THEN PUT THE "STOP/START" SWITCH TO "START" AGAIN. THE TAPE SHOULD REWIND TO LOAD POINT. FINALLY, PUT THE "ON LINE/OFF LINE" SWITCH TO "ON LINE".

TO DISMOUNT A TAPE, ONE MUST PUT THE "ON LINE/OFF LINE" SWITCH TO "OFF LINE", REWIND THE TAPE, AND THEN PUT THE "BRAKE RELEASE/LOAD" SWITCH TO "BREAK RELEASE". AFTER A FEW MOMENTS, ONE SHOULD OPEN THE DOOR, AND GENTLY WIND OFF THE TAPE TO THE LOWER REEL, REMOVE IT, CLOSE THE DOOR AND RETURN THE TAPE TO ITS CANNISTER.

6.2. MOUNTING DISCS

DISCS SHOULD BE HANDLED WITH EVEN GREATER CARE THAN MAGNETIC TAPES. WHEN NOT IN USE THEY SHOULD BE EITHER EXACTLY VERTICAL, OR EXACTLY HORIZONTAL SO THAT THEY WILL NOT WARP.

TO MOUNT A DISC, ONE STARTS WITH THE DISC OUT OF ITS RACK AND BAG AND WITH THE DRIVE FREE. ONE CAREFULLY OPENS THE DOOR OF THE DRIVE AND THEN SLIDES THE DISC IN HORIZONTALLY, WITH THE RAISED PORTION ON TOP POINTING TO THE REAR OF THE DRIVE, AND THE LABEL OF THE DISC DIRECTLY TO THE FRONT. NO SIGNIFICANT AMOUNT OF FORCE IS REQUIRED. IF ONE BENDS THE GUIDES, THE DRIVE MUST NOT BE USED. ONCE THE DISC IS IN PLACE, ONE CLOSES THE DOOR, AND MOVES THE "RUN/LOAD" SWITCH TO "RUN".

TO UNLOAD A DISC, MOVE THE "RUN/LOAD" SWITCH TO "LOAD" AND WAIT FOR THE "LOAD" LIGHT TO COME ON. THIS MAY TAKE A FEW MINUTES. THEN ONE OPENS THE DOOR OF THE DRIVE BY PULLING FORWARD AT THE TOP AND DOWN. THIS LEVERS THE PACK OFF THE SPINDLE. THEN PULL STRAIGHT OUT. THE PACK SHOULD BE RETURNED TO ITS BAG AND RACK AND THE DOOR OF THE DRIVE SHOULD BE CLOSED.

6.3. MOUNTING CARDS

CARDS ARE LOADED INTO THE CARD READER FACE DOWN, 12 EDGE UP, WITH THE CARD WEIGHT RESTING BEHIND THEM. ONE PRESSES THE READY BUTTON AND WAITS FOR THE READY LIGHT TO COME ON.

THE CARD READER SHOULD SHUT ITSELF OFF AFTER THE LAST CARD IS READ.

6.4. MOUNTING PAPER TAPE

THE ONLY SPECIAL PRECAUTION ABOUT MOUNTING PAPER TAPE IS TO BE CERTAIN THAT THE SPROCKET HOLES ARE OVER THE DRIVE WHEEL. THE DIRECTION OF FEED SHOULD BE MARKED ON THE READER.

6.5. MOUNTING PRINTER PAPER

INSTRUCTIONS FOR MOUNTING PRINTER PAPER ARE ON THE FRONT DOOR OF THE PRINTER. ONE SHOULD BE VERY CAREFUL TO ARRANGE THE PAPER SO THAT THE BLACK END-OF-PAGE MARK IS ON THE LEFT UNDERSIDE OF THE PAPER AS IT FEEDS OUT.

7. RUNNING DIAGNOSTICS

MOST DIAGNOSTICS ARE NOT ABLE TO RUN IN THE NORMAL OPERATING SYSTEM ENVIRONMENT. THEY MAY BE LOADED FROM THE "DEC DIAGNOSTIC DISC PACK", PAPER TAPE OR MAGNETIC TAPE. FOR DISC OR MAGNETIC TAPE, ONE BOOTSTRAPS THE MEDIUM, AND THEN TYPES THE NAME OF THE DIAGNOSTIC. FOR PAPER TAPE, ONE LOADS THE "ABSOLUTE LOADER" (SEE THE "DIGITAL PDP11 PROGRAMMING CARD") VIA THE "BOOTSTAP LOADER", AND THEN STARTS THE DIAGNOSTIC. THE MOST COMMON STARTING ADDRESS IS 200.

8. CRYSNET TERMINAL PROGRAMS AND LIBRARIES

WRITEUPS OF THE PROGRAMS SUPPLIED AS PART OF THE CRYSNET TERMINAL SOFTWARE ARE DESCRIBED IN DETAIL IN APPENDIX 1. THE EXACT PROGRAMS AT ANY INSTALLATION WILL VARY, SINCE IT IS VERY EASY TO INTRODUCE NEW CODE. AMONG THE PROGRAMS AND LIBRARIES AVAILABLE ARE THE FOLLOWING:

FTNLIB.OBJ

THIS IS A MODIFIED FORM OF THE STANDARD DEC FORTRAN OBJECT TIME SYSTEM WITH THE FOLLOWING ROUTINES ADDED:

BUFFER - SUBROUTINES FOR ASYNCHRONOUS I/O (BUFFEI/BUFFEO)
IOCHEK - A SUBROUTINE FOR ASYNCHRONOUS I/O
DELFIL - A SUBROUTINE TO DELETE A FILE FROM FORTRAN

FDPLIB.OBJ

THIS IS A MODIFIED VERSION OF THE VECTOR GENERAL FDP VERSION 6 LIBRARY WITH SOFTWARE TEXT ROUTINES AND THREE-DIMENSIONAL LINE AND POSITION ROUTINES (TLINE AND TPOSTN).

PLTLIB.OBJ

THIS IS A LIBRARY OF VERSATEC PLOTTING SUBROUTINES. PLOT IMAGES ARE BUILT UP ON A DISC BUFFER AND THEN COPIED OUT TO THE VERSATEC.

VECTOR.OBJ

THIS IS A LIBRARY OF ROUTINES FOR VECTOR MANIPULATIONS. IT GREATLY ENHANCES THE READABILITY AND MAINTAINABILITY OF CODE. A VERSION OF VECTOR IS ALSO AVAILABLE FOR THE CDC 6600 AND 7600 (SEE P. IV-13).

V3DLIB.OBJ

THIS IS AN ADDITIONAL LIBRARY FOR THE VECTOR GENERAL ALLOWING EXTENSIVE THREE-DIMENSIONAL OPERATIONS.

AMD.LDA

THIS IS THE COMMUNICATIONS PROGRAM FOR USE AGAINST CDC CENTRAL SITES. IT SIMULATES A CDC 200 SERIES USER TERMINAL (ASCII OR BCD), AND INCLUDES CODE FOR THE TRANSMISSION OF NON-STANDARD TAPE FORMATS. THE PROTOCOL SUPPORTS LINES FROM 2000 BAUD THROUGH 9600 BAUD WITH SYNCHRONOUS MODEMS.

S4010.LDA

THIS IS A PROGRAM TO SIMULATE A TECTRONIX 4010, USING THE VECTOR GENERAL DISPLAY. INPUT AND OUTPUT MAY BE DOS FILES IN PLACE OF PAPER TAPE.

ALLD.LDA

THIS IS A PROGRAM TO COMPUTE MOLECULAR GEOMETRY. DISTANCES, ANGLES, TORSION ANGLES AND PLANES MAY BE COMPUTED.

BUILDR.LDA

THIS IS A MOLECULAR-MODEL BUILDING PROGRAM WHICH ACCEPTS DISTANCES, ANGLES AND TORSION ANGLES TO PRODUCE A MODEL.

CART.LDA

THIS IS A PROGRAM TO COMPUTE CARTESIAN COORDINATES RELATIVE TO ANY GIVEN PLANE.

CALCSF.LDA

THIS PROGRAM CALCULATES STRUCTURE FACTORS.

CONTUR.LDA

THIS IS A PROGRAM TO CONTOUR ELECTRON-DENSITY MAPS AND PATTERSON FUNCTIONS ON THE VERSATEC PLOTTER. THE MAP INPUT IS GENERATED AS AN OPTION OF THE PROGRAM FOURR.

DECAY.LDA

THIS PROGRAM CALCULATES THE DECAY CURVE FOR STANDARD INTENSITY DATA AND PLOTS THE CURVE ON THE VERSATEC PLOTTER.

EXTCAL.LDA

THIS PROGRAM CALCULATES A SECONDARY EXTINCTION COEFFICIENT USING THE FILE OF OBSERVED AND CALCULATED STRUCTURE FACTORS WRITTEN BY THE STRUCTURE FACTOR CALCULATION PROGRAM CALCSF.

ELLIPS.LDA

THIS IS A PROGRAM TO COMPUTE ATOMIC VIBRATION PARAMETERS FROM TEMPERATURE FACTORS AND TO DISPLAY THE RESULTS ON THE VECTOR GENERAL DISPLAY.

FACES.LDA

FACES IS AN AID IN DEFINING CRYSTAL GEOMETRY BY CALCULATING EQUATIONS OF CRYSTAL-SURFACE PLANES AND THEIR DISTANCES FROM THE ORIGIN. PROGRAM FACES PROVIDES A DISPLAY OF BOTH THE COMPUTED AND MEASURED CRYSTAL FOR COMPARISON. A VERSION OF FACES IS ALSO AVAILABLE FOR THE CDC 6600 AND 7600 (SEE P IV-8).

FOURR.LDA

THIS IS A PROGRAM TO BE USED FOR THE COMPUTATION OF CRYSTALLOGRAPHIC FOURIER SYNTHESES. THIS VERSION OF THE PROGRAM IS INTENDED FOR USE FOR

TRICLINIC, MONOCLINIC OR ORTHORHOMBIC SPACE GROUPS.

HKLTRN.LDA

THIS PROGRAM TRANSFORMS THE H, K, L INDICES OF A SET OF REFLECTION DATA SO THAT AXES MAY BE INTERCHANGED OR LATTICE CENTERING CHANGED.

LISTFC.LDA

THIS PROGRAM PRODUCE A COMPACT LISTING OF F OBS AND F CALC. THE REFLECTION INPUT IS THAT GENERATED BY CALCSF AND RESIDES ON FOURR.DAT.

MSRED.LDA

THIS PROGRAM CALCULATES STRUCTURE AMPLITUDES FROM RAW DATA.

PARAML.LDA

THIS PROGRAM PRODUCES A COMPACT LISTING OF FINAL ATOMIC PARAMETERS.

PECKER.LDA

THIS PROGRAM PICKS OUT AND LISTS THOSE PEAKS FROM A PREVIOUSLY RUN FOURIER EQUAL TO OR GREATER THAN A GIVEN RHO VALUE.

PRJCTN.LDA

PRJCTN IS A PROGRAM FOR DISPLAY OF MOLECULES AS STICK BOND FIGURES ALLOWING FOR INTERACTIVE ROTATION ABOUT AXES. GEOMETRY CALCULATIONS AND PLOTTING ARE INCLUDED. LIMITED EDITING OF THE DISPLAY IMAGE IS PERMITTED. A VERSION OF PRJCTN TO PRODUCE CALCOMP PLOTS IS AVAILABLE FOR THE CDC 6600 AND 7600 (SEE P IV-11).

RSTD.LDA

THIS PROGRAM CHECKS STANDARD REFLECTIONS FROM DATA COLLECTIONS.

SANDA.LDA

THIS IS A PROGRAM TO COMPUTE INTRAMOLECULAR AND INTERMOLECULAR DISTANCES. A VERSION OF SANDA IS AVAILABLE FOR THE CDC 6600 AND 7600 (SEE P IV-12).

SCALER.LDA

THIS IS A PROGRAM TO COMPUTE THE SCALE AND TEMPERATURE FACTORS BY WILSON'S METHOD AND TO COMPUTE E'S AND OBTAIN ASSOCIATED STATISTICS.

STIPL.LDA

THIS IS A PROGRAM TO DISPLAY SPACE FILLING MODELS OF MOLECULES WITH STIPPLED SURFACES (HIDDEN SURFACES REMOVED).

9. INSTALLING AND MAINTAINING SYSTEMS

THE KEY USER MUST INSTALL AND MAINTAIN COPIES OF THE SYSTEM IN SOME COHERENT MANNER. IN A SYSTEM WITH ONE DISC DRIVE, USERS WILL BE SHARING SPACE ON A COMMON DISC. IN THAT CASE, THE KEY USER WILL ALSO HAVE TO ENSURE ENOUGH FREE SPACE ON THE DISC TO ALLOW USEFUL WORK TO BE DONE.

THE TWO PROGRAMS NEEDED FOR SUCH MAINTENANCE ARE "VERIFY" AND "ROLLIN". ALSO, WHEN THE DISC FILLS UP, FILES WILL HAVE TO BE SAVED ON TAPE AND DELETED BY THE PROGRAM "PIP".

9.1. INSTALLING A SYSTEM

CRYSNET SYSTEMS ARE USUALLY PROVIDED AS "ROLLIN" FORMAT TAPES. IN ORDER TO INSTALL SUCH A TAPE ONTO A DISC, ONE MUST START WITH A DISC FREE FOR WRITING ON THE DRIVE, AND THE ROLLIN TAPE MOUNTED AND ON LINE. ONE MUST THEN BOOTSTRAP THE TAPE. FOR A MR11-DB THE BOOTSTARP ADDRESS IS 773136. FOR A BM873-YA THE BOOTSTRAP ADDRESS IS 773050. FOR A BM873-YB THE BOOTSTRAP ADDRESS IS 773110. THE MESSAGE "ROLLIN V7" AND A "#" SHOULD APPEAR ON THE CONSOLE. ONE THEN TYPES

```
DK:/FO<MT0:CNET/RW
```

FOLLOWED BY A CARRIAGE RETURN (NEW LINE ON SOME MACHINES). THIS WILL CAUSE THE PROGRAM TO FORMAT THE DISC PACK AND THEN COPY A FULL DISC IMAGE ONTO THE DISC. THE PRIOR CONTENTS OF THE DISC WILL BE LOST. WHEN THE "#" NEXT APPEARS, ONE MAY BOOTSTRAP THE DISC.

9.2. MAINTAINING A SYSTEM

AT REGULAR INTERVALS, THE KEY USER SHOULD ROLL A BACKUP COPY OF THE CURRENT SYSTEM TO TAPE, ROTATING AMONG AT LEAST THREE TAPES, AND AT LEAST TWO DISC PACKS. TO DO SO, THE KEY USER SHOULD BOOTSTRAP A COPY OF ROLLIN, EITHER FROM A ROLLIN TAPE AS ABOVE, OR FROM THE COPY THAT IS KEPT ON THE SYSTEM DISC. IN THE SECOND CASE, ON MUST LOGIN UNDER "1,1" AND RUN THE PROGRAM "CILUS". ONE THEN TYPES

```
ROLLIN.CIL/BO
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WHICH WILL LOAD ROLLIN. ONE THEN MOUNTS A TAPE WHICH MAY BE OVERWRITTEN, WITH A WRITE RING INSTALLED, AND TYPES

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MT0:CNET<DK:/RW/DA:DD-MMM-YY
```

FOLLOWED BY A CARRIAGE RETURN, WHERE "DD" IS THE TWO DIGITS OF THE CURRENT DAT, "MMM" IS THE THREE LETTER ABBREVIATION OF THE CURRENT

MONTH, AND "YY" IS THE LAST TWO DIGITS OF THE CURRENT YEAR. THE ENTIRE DISC WILL BE COPIED TO THE TAPE.

PERIODICALLY THE KEY USER SHOULD RUN THE PROGRAM "VERIFY" TO INSURE THAT THE DISC HAS NOT BEEN CORRUPTED. THE SEQUENCE

```
RU VERIFY
SY
FIX
```

WILL DETECT AND CORRECT ERRORS AND PRINT THEM ON THE PRINTER. SEE THE "DOS/BATCH HANDBOOK" FOR MORE DETAILS.

THE SWITCH "/FR" UNDER PIP ALLOWS ONE TO CHECK FOR AVAILABLE SPACE. IT IS EXTREMELY DIFFICULT TO RUN WITH FEWER THAN 300 BLOCKS FREE. WHEN THAT HAPPENS, EITHER USERS MUST REMOVE SOME OF THEIR FILES, OR THE KEY USER HAS TO DO IT FOR THEM. IT IS BAD PRACTICE TO DELETE FILES WITHOUT FIRST COPYING THEM TO TAPE. SUCH TAPES SHOULD BE KEPT AS LONG AS POSSIBLE. USERS TEND TO DISCOVER A NEED FOR SUCH FILES JUST AFTER THEY HAVE BEEN PERMANENTLY LOST.

9.3. RECORD KEEPING

THE KEY USER MUST ASSUME RESPONSIBILITY FOR MAINTAINING CERTAIN ESSENTIAL RECORDS ABOUT THE TERMINAL. FOR THE USERS, HE SHOULD MAINTAIN A LIST OF ASSIGNED UIC'S, A MACHINE LOG-BOOK, AND A SIGN-UP BOOK. EACH OF THESE MAY BE IN WHATEVER FORM SUITS THE INSTALLATION, BUT SOME PROVISION MUST BE MADE IN THE LOG-BOOK FOR RECORDING THE TIMES OF USE AND INITIALS OF EACH USER. ONE MUST ALSO MAINTAIN MAINTENANCE RECORDS FOR EACH PART OF THE TERMINAL. THIS MAY BE DONE IN THE SAME LOG-BOOK, OR IN A SEPARATE MAINTENANCE LOG-BOOK. ONE MUST ALSO KEEP A RECORD OF ALL MAINTENANCE CONTRACTS, AND A LIST OF TELEPHONE NUMBERS OF THE PROPER SERVICE PERSONS FOR THE VARIOUS COMPONENTS OF THE TERMINAL.

IV. CENTRAL SITE OPERATIONS

THE CRYSNET TERMINALS COMMUNICATE WITH THE CDC CYBER 70/76 COMPUTING SYSTEM AT THE BNL CSCF. THE CYBER 70/76 SUPPORTS BOTH BATCH AND INTERACTIVE JOB PROCESSING. AN EXTENSIVE LIBRARY OF CRYSTALLOGRAPHIC PROGRAMS IS MAINTAINED AT THE CSCF, AND THIS SOFTWARE HAS BEEN ADAPTED TO ALLOW CONVENIENT USE FROM THE CRYSNET TERMINALS. THE TERMINALS ALSO PROVIDE ACCESS TO THE PROTEIN DATA BANK, A LIBRARY OF MACROMOLECULAR STRUCTURAL DATA STORED AT THE CSCF.

PROSPECTIVE CRYSNET USERS SHOULD CONTACT THE BNL APPLIED MATHEMATICS DEPARTMENT. INQUIRIES REGARDING THE USE OF THE CSCF SHOULD BE DIRECTED TO

MR. D. A. RAVENHALL
APPLIED MATHEMATICS DEPARTMENT
BUILDING 515
BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973

A BOOKLET ENTITLED "A GUIDE TO THE USE OF BROOKHAVEN NATIONAL LABORATORY'S CENTRAL SCIENTIFIC COMPUTING FACILITY BY OTHER MEMBERS OF THE SCIENTIFIC COMMUNITY" IS AVAILABLE FROM THE APPLIED MATHEMATICS DEPARTMENT.

I. HARDWARE

THE CSCF IS EQUIPPED WITH A CDC 7600 AND TWO CDC 6600'S. THE 7600 HAS 65,536 60-BIT WORDS OF SMALL CORE MEMORY (SCM) AND 512,000 WORDS OF LARGE CORE MEMORY (LCM). ONE 6600 HAS 98,306 60-BIT WORDS OF CENTRAL MEMORY AND THE OTHER HAS 65,536 WORDS OF CENTRAL MEMORY. THE 6600'S SHARE 1.5 MILLION WORDS OF EXTENDED CORE STORAGE (ECS). THE 6600'S SERVE AS I/O STATIONS FOR THE 7600. GENERALLY, THE INTERCOM SYSTEM, WHICH SUPPORTS REMOTE-JOB ENTRY AND INTERACTIVE ACCESS, IS RUN ON THE LARGER OF THE TWO 6600'S. THE 7600 HAS 12 CDC 844 DISC DRIVES (APPROXIMATELY 140 MILLION WORDS CAPACITY). BINARIES OF ALL CENTRAL-SITE CRYSTALLOGRAPHIC PROGRAMS ARE CURRENTLY MAINTAINED ON TWO PRIVATE 844 DISC PACKS WHICH BELONG TO THE CHEMISTRY DEPARTMENT. THE 6600'S EACH HAVE TWO CDC 6603 DISC DRIVES. THESE 6603'S, WHICH PROVIDE APPROXIMATELY 140 MILLION WORDS CAPACITY PER 6600, ARE SOON TO BE REPLACED WITH 844 DRIVES. THE 6600'S ALSO SHARE EIGHT CDC 841 DISC DRIVES (APPROXIMATELY 21 MILLION WORDS CAPACITY). SEVEN AND NINE-TRACK MAGNETIC TAPE DRIVES ARE AVAILABLE ON-LINE TO THE 6600'S. THESE DRIVES ARE USED BY THE 6600'S TO STAGE TAPE FILES TO THE 7600. TAPES MAY BE WRITTEN AT DENSITIES OF 200, 556, OR 800 BPI (SEVEN TRACK) AND 800 OR 1600 BPI (NINE TRACK). INTERCOM REMOTE COMMUNICATIONS ARE SUPPORTED THROUGH CDC 7077-791 FRONT-END PROCESSORS.

THE CRYSNET TERMINALS NORMALLY ARE HANDLED ON DIRECT-DIAL TELEPHONE LINES. SYNCHRONOUS COMMUNICATIONS SPEEDS FROM 2000 TO 4800 BAUD ARE POSSIBLE WITH DIRECT-DIAL LINES (9800 BAUD REQUIRES A DEDICATED CHANNEL). THE FRONT-END PROCESSORS ARE ALSO CAPABLE OF HANDLING

INTERACTIVE KEYBOARD TERMINALS ON DIRECT-DIAL LINES AT SPEEDS OF 110 AND 300 BAUD (ASYNCHRONOUS). TELEPHONE NUMBERS FOR COMMUNICATIONS PORTS ARE:

2000 BAUD	516-345-2659	(FOUR PORTS)	
4800 BAUD	516-345-4146 OR 212-895-2141	(TWO PORTS)	
300 BAUD	516-345-2635	(18 PORTS)	
110 BAUD	516-345-2651	(SIX PORTS)	

TO CALL 516-345-XXXX NUMBERS ON FTS, DIAL 664-XXXX.

FOR PLOTTING, THE CSCF HAS AVAILABLE AN OFF-LINE, MAGNETIC-TAPE DRIVEN CALCOMP 835, WHICH PROVIDES BOTH 35MM FILM STRIP AND PAPER PLOTTING.

AN III FR-80 COMPUTER OUTPUT MICROFILM RECORDER IS SCHEDULED TO BE ACQUIRED BY THE CSCF IN JUNE 1976.

2. SYSTEM SOFTWARE

OPERATING SYSTEMS IN USE ARE CDC SCOPE 2.1 ON THE 7600 AND SCOPE 3.4 ON THE 6600'S. INTERCOM 4.2 IS SUPPORTED UNDER SCOPE 3.4. THE I/O STRUCTURE IS THAT PROVIDED BY THE CDC RECORD MANAGER. MAJOR LANGUAGES SUPPORTED ARE FORTRAN (BOTH FTN AND RUN COMPILERS), COBOL, ALGOL, BASIC, AND THE ASSEMBLY LANGUAGE COMPASS. FOR DETAILED INFORMATION REGARDING SYSTEM SOFTWARE, THE READER IS REFERRED TO THE FOLLOWING CDC PUBLICATIONS:

7600

SCOPE 2.1 REFERENCE MANUAL (PUBLICATION NUMBER 60342600)
SCOPE 2.1 USER'S GUIDE (60372600)

7600 AND 6600

COMPASS 3 REFERENCE MANUAL (60360900)
FORTRAN EXTENDED 4 REFERENCE MANUAL (60305600)
LOADER REFERENCE MANUAL (60344200)
RECORD MANAGER REFERENCE MANUAL (60307300)

6600

INTERCOM 4 REFERENCE MANUAL (60307100)
SCOPE 3.4 REFERENCE MANUAL (60307200)
SCOPE 3.4 USER'S GUIDE (60358700)

3. CRYSTALLOGRAPHIC PROGRAMS

THE LIBRARY OF CRYSTALLOGRAPHIC PROGRAMS IS AVAILABLE ON BOTH THE 6600'S AND ON THE 7600. AS MENTIONED IN SECTION 1 ABOVE, EXECUTABLE

BINARIES FOR THE 7600 ARE STORED ON TWO PRIVATE DISC PACKS BELONGING TO THE BNL CHEMISTRY DEPARTMENT. FOR THE 6600, BINARIES ARE STORED ON MAGNETIC TAPE, AND MAY BE ATTACHED TO THE USER'S JOB WITH THE UTILITY PROGRAM ACCESS. SOURCE CODE FOR ALL PROGRAMS IS AVAILABLE IN THE FORM OF A CDC UPDATE FILE ON MAGNETIC TAPE C206, AND AS A PERMANENT FILE NAMED OLDPL ON ONE OF THE PRIVATE DISC PACKS (7600 ONLY). PERMANENT FILES CONTAINING SOURCE CODE OR BINARIES FOR CRYSTALLOGRAPHIC PROGRAMS ARE CATALOGED UNDER ID=CPROGS, EXCEPT FOR FILES PERTAINING SPECIFICALLY TO THE PROTEIN DATA BANK, WHICH ARE CATALOGED UNDER ID=PDB. THE TWO CHEMISTRY PRIVATE PACKS ARE IDENTIFIED BY SN=CHEM AND SN=ISTRY, RESPECTIVELY.

SAMPLE JOB SET-UPS, SHOWING CONTROL-STATEMENT SEQUENCES FOR EXECUTION OF CRYSTALLOGRAPHIC PROGRAMS, FOLLOW:

7600

```
1.  JOB01,CP70,YD1,T77,TP0,EC60.  SAMPLE 7600 JOB
2.  ACCOUNT,MURPHY,899.
3.  MOUNT,VSN=CHEM01,SN=CHEM.
4.  ATTACH,TAPE1,DATA,ID=MURPHY.
5.  REQUEST,TAPE3,*PF.
6.  ATTACH,AVSORT,ID=CPROGS,SN=CHEM.
7.  FTN,R=3,A,EL=A,SYSEDIT,OPT=2.
8.  REWIND,LGO.
9.  COPYL,AVSORT,LGO,PROG.
10. PROG.
11. REWIND,TAPE3.
12. CATALOG,TAPE3,RESULTS,ID=MURPHY,XR=MURPHY,RP=14,AC=899.
13. REWIND,TAPE3.
14. 7/8/9
15. SOURCE CODE FOR SUBROUTINES TO BE REPLACED
16. 7/8/9
17. DATA
18. END-OF-FILE
```

NOTES

1. JOB STATEMENT: CP70 FOR EXECUTION ON THE 7600
   YD1 FOR MOUNTING OF A PRIVATE DISC PACK
   T77 TIME LIMIT 77 (OCTAL) SECONDS
   TP0 NO STAGING OF MAGNETIC TAPE FILES.
   .... OMIT IF STAGED FILES ARE PRESENT.
   EC60 TO ALLOCATE 60,000 (OCTAL) WORDS OF LCM STORAGE.

2. ACCOUNT STATEMENT MUST GIVE USER'S NAME AND ACCOUNT NUMBER.

3. MOUNT STATEMENT TO MOUNT THE PRIVATE PACK IDENTIFIED BY SN=CHEM. TO MOUNT THE OTHER PACK, USE MOUNT,VSN=ISTRY1,SN=ISTRY. IN THIS CASE REPLACE SN=CHEM BY SN=ISTRY ON CONTROL STATEMENT 6.

4. THE DATA FOR THIS CALCULATION ARE ASSUMED TO BE STORED ON A PERMANENT FILE NAMED DATA UNDER ID=MURPHY.

5. THIS CONTROL STATEMENT ASSIGNS FILE TAPE3 TO A PERMANENT-FILE DEVICE.

6. ATTACH STATEMENT TO ATTACH THE BINARY CODE FOR PROGRAM AVSORT.

7. FTN STATEMENT INCLUDED ONLY IF SUBROUTINES ARE TO BE RECOMPILED.

8. REWIND STATEMENT IS REQUIRED AT THIS POINT IF SUBROUTINES ARE TO BE RECOMPILED.

9. COPYL CREATION OF BINARY WITH RECOMPILED SUBROUTINES INCLUDED ONLY IN CONJUNCTION WITH FTN STATEMENT.

10. EXECUTION STATEMENT WOULD BE AVSORT., IN THE ABSENCE OF CONTROL STATEMENTS 7-9.

11. REWIND FILE TAPE3, WHICH CONTAINS RESULTS OF THIS CALCULATION, BEFORE SAVING AS A PERMANENT FILE. IT IS ALWAYS A GOOD PRACTICE TO REWIND A FILE BEFORE CATALOGING IT.

12. SAVE TAPE3 AS A PERMANENT FILE WITH THE NAME RESULTS UNDER ID=MURPHY, WITH PASSWORD MURPHY AND RETENTION PERIOD 14 DAYS. ALTERNATIVELY, TAPE3 MIGHT BE SAVED AS A POST-STAGED MAGNETIC TAPE FILE. IN THIS CASE, TP0 WOULD BE OMITTED ON THE JOB STATEMENT.

13. A REWIND AFTER CATALOGING IS GOOD STANDARD PRACTICE.

14. SCOPE END OF RECORD - MULTIPUNCHED 7/8/9 IN COLUMN 1

15. INCLUDE ONLY IF SUBROUTINES ARE TO BE RECOMPILED.

16. INCLUDE ONLY IF SUBROUTINES ARE TO BE RECOMPILED.

17. SEE DETAILED PROGRAM WRITEUPS (APPENDIX 2) FOR DESCRIPTION OF DATA.

18. FOR JOBS SUBMITTED IN THE FORM OF CARD DECKS FROM THE CRYSNET TERMINALS, THE APPROPRIATE END-OF-FILE IS A DEC END-OF-FILE CARD WITH MULTIPUNCHED 12/11/0/1/6/7/8/9 IN COLUMN 1. THIS IS EQUIVALENT TO THE SCOPE END-OF-FILE CARD WITH MULTIPUNCHED 6/7/8/9 IN COLUMN 1.

6600

```
1.  JOB02,T77,NT2,MT1,EC60.   SAMPLE 6600 JOB
2.  ACCOUNT,MURPHY,899.
3.  ATTACH,ACCESS,ID=CPROGS.
4.  ACCESS,AVSORT,ID=CPROGS.
5.  FTN,R=3,A,EL=A,SYSEDIT,OPT=2.
6.  REWIND,LGO.
7.  COPYL,AVSORT,LGO,PROG.
8.  REQUEST,TAPE1,E,HD,VSN=N10001,NORING.
9.  REQUEST,TAPE2,N,HD,VSN=N10002,RING.
10. PROG.
11. 7/8/9
12. SOURCE CODE FOR SUBROUTINES TO BE REPLACED
13. 7/8/9
14. DATA
```

15. END-OF-FILE

NOTES

1. JOB STATEMENT: MT1 FOR USE OF AN ON-LINE SEVEN-TRACK MAGNETIC TAPE. THIS TAPE MAY BE NEEDED BY UTILITY PROGRAM ACCESS. NT2 FOR USE OF TWO ON-LINE NINE-TRACK MAGNETIC TAPES FOR DATA FILES. GENERALLY, THE USE OF TAPES FOR LARGE DATA FILES IS PREFERRED TO THE USE OF PERMANENT FILES, ESPECIALLY ON THE 6600 WHERE FILE SPACE OFTEN IS VERY TIGHT, AND PERMANENT FILE CHARGES MAY BE QUITE HIGH.

3. ATTACH THE UTILITY PROGRAM ACCESS.

4. ACCESS WILL ATTACH THE BINARY CODE FOR PROGRAM AVSORT, IF A PERMANENT FILE WITH THIS NAME APPEARS IN THE SYSTEM DIRECTORY. IF NO SUCH FILE EXISTS, ACCESS WILL BRING A COPY IN FROM TAPE AND CREATE A PERMANENT FILE WITH NULL RETENTION PERIOD.

8. REQUEST THE DATA TAPE N10001. THIS IS A STANDARD SCOPE (RT=S) NINE-TRACK, 800 BPI, LABELLED TAPE.

9. REQUEST TAPE N10002 ON WHICH THE RESULTS WILL BE WRITTEN. THIS WILL BE WRITTEN IN THE SAME FORMAT AS TAPE N10001.

AS HAS BEEN MENTIONED ABOVE, SOURCE CODE FOR ALL CRYSTALLOGRAPHIC PROGRAMS IS AVAILABLE AS A PROGRAM LIBRARY FOR USE WITH CDC UPDATE ON BOTH THE 6600'S AND THE 7600. TO ACCESS THE PROGRAM LIBRARY USE THE FOLLOWING STATEMENTS:

```
7600:   ATTACH,OLDPL,ID=CPROGS,SN=CHEM.
6600'S: REQUEST,OLDPL,E,HI,VSN=C206.    (SCOPE RT=S TAPE)
```

CRYSNET USERS MAY WISH TO PRINT LARGE JOBS AT THE CSCF, AND ARRANGE TO HAVE THE OUTPUT MAILED. IN THIS CASE, THE FIRST THREE CHARACTERS OF THE JOB'S NAME SHOULD BE D77. INSERTING ONE OF THE STATEMENTS

```
DISPOSE,OUTPUT,*PR=C,ST=MFA.    (FOR 7600 JOBS)
DISPOSE,OUTPUT,*PR=C.    (FOR 6600 JOBS)
```

AFTER THE ACCOUNT CARD WILL CAUSE A JOB TO PRINT AT THE CSCF. ALTERNATIVELY, LONG JOBS APPEARING IN THE TERMINAL'S OUTPUT QUEUE CAN BE DIVERTED, BY EXECUTING THE INTERCOM COMMAND

```
DIVERT,AA.
```

WHERE AA STANDS FOR THE LAST TWO CHARACTERS OF THE JOB'S NAME. THE D77 DESIGNATION CAUSES A JOB TO BE DELIVERED TO THE DATA SERVICES GROUP, WHO ARE RESPONSIBLE FOR MAILING OUTPUT. THE USER SHOULD INSERT HIS MAILING ADDRESS IN HIS DAYFILE WITH COMMENT STATEMENTS.

THE BROOKHAVEN LIBRARY OF CRYSTALLOGRAPHIC PROGRAMS CONTAINS AN EXTENSIVE SET OF ROUTINES FOR DATA ACQUISITION AND INITIAL PROCESSING, STRUCTURE SOLUTION AND REFINEMENT, AND STRUCTURE ANALYSIS. THE GENERAL LOGICAL FLOW OF MAJOR PROGRAMS IS INDICATED IN FIGURE IV-1. IN ADDITION TO THE PROGRAMS SHOWN IN THIS FIGURE, THE LIBRARY INCLUDES:

HERM - PROTEIN REFINEMENT PACKAGE (METHOD OF LOCAL CHANGE)
LEASTSQ - MULTIPLE ISOMORPHOUS REPLACEMENT PHASING PROGRAM
ORTRAN - RECIPROCAL SPACE FOURIER-TRANSFORM SEARCH

AND SEVERAL OTHER PROGRAMS OF LESS GENERAL APPLICATION. THE FOLLOWING UTILITY ROUTINES ARE ALSO AVAILABLE:

ACCESS - FILE RETRIEVAL UTILITY
EDIT - CONTEXT EDITOR UTILITY
RMCOPY - COPY UTILITY USING RECORD MANAGER
TYPIST - UTILITY DOCUMENTATION PROGRAM

A LIST OF THE COMPLETE CONTENTS OF THE LIBRARY IS GIVEN IN TABLE IV-1, AND A BRIEF DESCRIPTION OF INDIVIDUAL PROGRAMS FOLLOWS. DETAILED PROGRAM DOCUMENTATION IS AVAILABLE IN APPENDIX 2.

ABSOR

ABSOR IS A PROGRAM TO CALCULATE ABSORPTION CORRECTIONS FOR DATA FROM AN EULERIAN FOUR-CIRCLE GONIOMETER BY THE ANALYTICAL METHOD OF DEMEULENAER AND TOMPA. PROGRAM ABSOR READS REFLECTION SETTING ANGLES AND RAW INTENSITY DATA PRODUCED BY PROGRAM PROCK. THE CALCULATED ABSORPTION CORRECTIONS ARE SUBSEQUENTLY APPLIED BY PROGRAM CORDAT. PROGRAM ABSOR BREAKS THE CRYSTAL UP INTO HOWELLS POLYHEDRA, AND CALCULATES THE ABSORPTION CORRECTION BASED UPON THESE POLYHEDRA. ABSOR ALSO CALCULATES THE ABSORPTION-WEIGHTED MEAN PATH LENGTH THROUGH THE CRYSTAL AND THE UNIT VECTORS REQUIRED FOR COMPUTATION OF ANISOTROPIC EXTINCTION CORRECTIONS. SEVERAL CHECKS HAVE BEEN BUILT INTO THE PROGRAM TO INSURE THE ACCURACY OF THE CALCULATIONS AND TO NOTE CASES WHERE THIS ACCURACY MAY BECOME COMPROMISED. ABSOR IS THE BROOKHAVEN VERSION OF A PROGRAM BY TEMPLETON ET AL.

AVBANG

AVBANG IS A PROGRAM TO CALCULATE MEAN VALUES AND VARIANCES OF A SAMPLE POPULATION. THE PROGRAM IS OFTEN USED TO COMPUTE AVERAGES OF BOND DISTANCES AND ANGLES BUT MAY BE USED FOR OTHER QUANTITIES, SUCH AS TORSION ANGLES, DISPLACEMENTS FROM LEAST-SQUARES PLANES, ETC.

AVSORT

AVSORT IS A PROGRAM TO SORT AND AVERAGE EQUIVALENT REFLECTION DATA. PROGRAM AVSORT READS F**2 DATA PRODUCED BY PROGRAM BNLABS OR CORDAT, AND PREPARES A FILE SUITABLE FOR INPUT TO THE STRUCTURE FACTOR LEAST-SQUARES PROGRAM FLINUS. THE PROGRAM MAKES EXTENSIVE USE OF LCM (7600) OR ECS (6600). IT IS QUITE FLEXIBLE IN OPERATION, AND CAN HANDLE UP TO A TOTAL OF 25,000 REFLECTIONS, WITH MILLER INDICES UP TO 49. PROVISION IS MADE TO DEFINE ANY LAUE SYMMETRY, AND OPTIONALLY TO EXCLUDE EXTINCT

REFLECTIONS. STATISTICS ARE CALCULATED TO INDICATE THE DEGREE OF AGREEMENT AMONG SYMMETRY-RELATED REFLECTIONS.

BNLABS

BNLABS IS A PROGRAM TO CALCULATE AND APPLY LORENTZ, POLARIZATION, AND ABSORPTION CORRECTIONS TO DATA FROM AN EULERIAN FOUR-CIRCLE DIFFRACTOMETER. ABSORPTION-WEIGHTED MEAN PATH LENGTHS AND UNIT VECTORS NEEDED IN THE COMPUTATION OF EXTINCTION CORRECTIONS ARE ALSO CALCULATED. PROGRAM BNLABS READS REFLECTION SETTING ANGLES AND RAW INTENSITY DATA PRODUCED BY PROGRAM PROCK. F**2 VALUES ARE OUTPUT IN A FORM SUITABLE FOR INPUT TO THE SORTING AND AVERAGING PROGRAM AVSORT, OR MAY BE USED DIRECTLY WITH THE STRUCTURE FACTOR LEAST-SQUARES REFINEMENT PROGRAM FLINUS. THE ABSORPTION CORRECTION IS COMPUTED BY DIVISION OF THE CRYSTAL INTO A GAUSSIAN GRID WITH THE NUMBER OF GRID POINTS SPECIFIED BY THE USER. A GRID OF UP TO 5000 POINTS MAY BE SPECIFIED. THE NUMERICAL INTEGRATION MAY BECOME QUITE TIME-CONSUMING FOR LARGE GRIDS, AND THEREFORE IN THE CASE OF CRYSTALS WITH SEVERE ABSORPTION, PROGRAM ABSOR WHICH CALCULATES ABSORPTION CORRECTIONS BY AN ANALYTICAL METHOD, IS PREFERRED OVER PROGRAM BNLABS.

COMPARE

PROGRAM COMPARE WILL CARRY OUT STATISTICAL COMPARISONS OF EXPERIMENTAL RESULTS. TESTS USED ARE FULL AND HALF-NORMAL PROBABILITY PLOTS, CHI-SQUARE, AND CONTRASTS. THE PROGRAM MAY BE USED TO COMPARE TWO SETS OF ATOMIC PARAMETERS (E.G. X-RAY AND NEUTRON DIFFRACTION RESULTS) OR TO COMPARE TWO SETS OF STRUCTURE FACTORS (E.G. FOBS AND FCALC). IT IS ALSO POSSIBLE TO CARRY OUT COMPARISONS BETWEEN ALL POSSIBLE PAIR-WISE COMBINATIONS OF UP TO SEVEN SETS OF ATOMIC PARAMETERS OR OTHER QUANTITIES OF INTEREST.

COORD

COORD IS A PROGRAM TO PRODUCE PUBLISHABLE LISTINGS OF ATOMIC PARAMETERS. THIS PROGRAM ACCEPTS ATOMIC PARAMETERS EITHER ON PUNCHED CARDS OR A FILE WRITTEN BY THE FUNCTION AND ERROR PROGRAM FREDFUN. STANDARD DEVIATIONS, IF SUPPLIED, ARE LISTED WITH THE PARAMETERS. PROVISION IS MADE FOR MERGING TWO ATOMIC PARAMETER FILES, AND FOR CHANGING THE ATOM NAMES GIVEN THEREIN.

CORDAT

CORDAT IS A PROGRAM TO APPLY LORENTZ, POLARIZATION, COUNTER DEAD-TIME AND ABSORPTION CORRECTIONS TO OBTAIN PROPERLY SCALED F**2 VALUES FROM RAW INTENSITY DATA OUTPUT BY PROGRAM PROCK. LORENTZ, POLARIZATION AND COUNTER DEAD-TIME CORRECTIONS ARE CALCULATED BY PROGRAM CORDAT, WHEREAS ABSORPTION CORRECTIONS ARE PASSED FROM PROGRAM ABSOR. THUS, IF NO ABSORPTION CORRECTIONS ARE PERFORMED (OR CALCULATIONS OF MEAN PATH LENGTHS AND UNIT VECTORS USED TO COMPUTE EXTINCTION CORRECTIONS), IN DATA REDUCTION ONE CAN PASS DIRECTLY FROM PROGRAM PROCK TO PROGRAM CORDAT. IF ABSORPTION OR EXTINCTION CORRECTIONS ARE NEEDED, ONE USES IN ADDITION PROGRAM ABSOR. (SEE FIGURE IV-1A). THE OUTPUT OF PROGRAM CORDAT IS SUITABLE FOR INPUT TO THE SORTING AND AVERAGING PROGRAM AVSORT, OR MAY BE USED DIRECTLY IN LEAST-SQUARES REFINEMENTS WITH

PROGRAM FLINUS.

DECOL

DECOL IS A PROGRAM TO DECOLLATE POOL TAPES WRITTEN AT THE REACTOR EXPERIMENTAL CONTROL FACILITY (RECF). STEP-SCAN PROFILE DATA ARE PRODUCED BY THE NEUTRON AND X-RAY DATA ACQUISITION SYSTEM (NEXDAS) THAT RUNS THE FOUR-CIRCLE DIFFRACTOMETERS AT THE HIGH FLUX BEAM REACTOR (HFBR). DECOL SEPARATES DATA WHICH ARE INTERMIXED ON THE POOL TAPES FROM DIFFERENT EXPERIMENTAL STATIONS AT THE HFBR, AND PRODUCES SEPARATE FILES FOR EACH USER. THESE FILES ARE SUITABLE FOR INPUT TO PROGRAM PROCK, WHICH CALCULATES INTEGRATED INTENSITIES FROM STEP-SCAN PROFILE DATA.

DISCOR

PROGRAM DISCOR IS USED TO OBTAIN BOND DISTANCES CORRECTED FOR EFFECTS OF THERMAL MOTION ACCORDING TO THE METHOD OF BUSING AND LEVY. THE UNCORRECTED AND THE 'LOWER-BOUND' (MINIMUM), 'UPPER-BOUND' (MAXIMUM) CORRECTED BOND DISTANCES, ARE CALCULATED ALONG WITH THE CORRECTED DISTANCE ASSUMING UNCORRELATED MOTION OF THE BONDED ATOMS.

FACES

FACES IS A PROGRAM USED AS AN AID IN DEFINING CRYSTAL GEOMETRY. THE PROGRAM STARTS WITH COORDINATES OF CRYSTAL VERTICES, AND CALCULATES EQUATIONS OF CRYSTAL SURFACE PLANES AND THEIR DISTANCES FROM THE ORIGIN. THUS, IT IS POSSIBLE TO MEASURE THE VERTEX COORDINATES DIRECTLY ON PHOTOMICROGRAPHS, AND CALCULATE EQUATIONS OF SURFACE PLANES. PROGRAM FACES MAY ALSO BE USED TO FIND UNWEIGHTED LEAST-SQUARES PLANES THROUGH COLLECTIONS OF ATOMS. THE PROGRAM CALCULATES THE INERTIA TENSOR (T) OF THE INPUT POINTS ABOUT THEIR CENTER OF MASS. THE BEST PLANE IS SOUGHT BY FINDING THE EIGENVECTOR OF THE LARGEST EIGENVALUE OF T.

FLINUS FLIN80

FLINUS IS A PROGRAM TO CALCULATE STRUCTURE FACTORS AND CARRY OUT FULL-MATRIX LEAST-SQUARES REFINEMENTS OF CRYSTAL STRUCTURES. PROGRAM FLINUS IS THE BROOKHAVEN MODIFICATION OF THE OAK RIDGE PROGRAM ORFLS. FLINUS IS THE STANDARD BNL VERSION AND ALLOWS UP TO 50 ATOMS AND UP TO 270 VARIABLES (558 PARAMETERS, INCLUDING THOSE NOT REFINED). FLIN80 IS A SPECIAL VERSION WHICH WILL TAKE UP TO 80 ATOMS, BUT WHICH IS LIMITED TO 262 VARIABLES. THESE PROGRAMS PERMIT INCLUSION OF ANOMALOUS DISPERSION AND ISOTROPIC AND ANISOTROPIC EXTINCTION CORRECTIONS.

FMUD1

FMUD1 IS A PROGRAM TO PERFORM LEAST-SQUARES REFINEMENTS OF UNIT CELL CONSTANTS AND ORIENTATION ANGLES, USING AS DATA SETTING ANGLES OF REFLECTIONS OBSERVED ON AN EULERIAN FOUR-CIRCLE GONIOMETER. PROVISION HAS BEEN MADE OPTIONALLY TO REFINE INSTRUMENT CONSTANTS (I.E. MECHANICAL ZEROES), AND TO ALLOW FOR SYMMETRY CONSTRAINTS ON CELL PARAMETERS. PROGRAM FMUD1 WILL ACCEPT UP TO A MAXIMUM OF 150 REFLECTIONS IN THE LEAST-SQUARES PROCEDURE. THE PROGRAM MAY ALSO BE USED TO CALCULATE SETTING ANGLES FOR A LIST OF REFLECTIONS, BASED ON THE

REFINED ORIENTATION ANGLES.

FREDFUN

FREDFUN IS THE BROOKHAVEN MODIFICATION OF THE OAK RIDGE FUNCTION AND ERROR PROGRAM ORFFE. PROGRAM FREDFUN WILL CALCULATE ESTIMATED STANDARD DEVIATIONS OF A VARIETY OF FUNCTIONS OF ATOMIC PARAMETERS (BOND DISTANCES, BOND ANGLES, DIHEDRAL ANGLES, ETC.), AND WILL COMPUTE LEAST-SQUARES PLANES. THE PROGRAM WILL ALSO GIVE ROOT MEAN SQUARE COMPONENTS OF THERMAL MOTION ALONG PRINCIPAL AXES, AND CORRECTIONS OF BOND LENGTHS FOR THERMAL MOTION. IN THE CALCULATION OF STANDARD DEVIATIONS, FREDFUN USES THE VARIANCE-COVARIANCE MATRIX OUTPUT BY PROGRAM FLINUS.

GENATM

GENATM IS A PROGRAM BY R. SHIONO DESIGNED TO DETERMINE NEW POSITIONS (ATOMIC SITES) GIVEN CERTAIN KNOWN POSITIONS AND CONSTRAINTS. THE PROGRAM'S MOST COMMON USE IS TO PREDICT HYDROGEN ATOM LOCATIONS FROM A KNOWLEDGE OF THE FRAMEWORK TO WHICH THE HYDROGEN ATOMS ARE BONDED. CONSTRAINTS MAY BE SPECIFIED IN TERMS OF BOND ANGLES AND TORSION ANGLES, OR NEW POSITIONS MAY BE DEFINED TO LIE ALONG A SPECIFIED INTER-ATOMIC VECTOR, OR NORMAL TO A PLANE.

HERM

HERM IS THE BROOKHAVEN VERSION OF PROGRAM REFINE2 BY J. HERMANS ET AL. FOR MODEL BUILDING AND ENERGY MINIMIZATION OF PROTEIN STRUCTURES. THE PROGRAM ADJUSTS A GIVEN SET OF COORDINATES OF A PROTEIN TO OBTAIN AN APPROXIMATELY IDEALIZED STRUCTURE. DURING MODEL BUILDING, BOND LENGTHS, BOND ANGLES AND DIHEDRAL ANGLES ARE IDEALIZED BY THE METHOD OF LOCAL CHANGE, IN WHICH ONE ATOM IS MOVED AT A TIME. SEVERAL PASSES MAY BE MADE THROUGH THE ENTIRE MOLECULE. FOR ENERGY MINIMIZATION, ENERGY CONTRIBUTIONS FOR DEFORMATION OF BOND LENGTHS, BOND ANGLES, AND FIXED DIHEDRAL ANGLES ARE MINIMIZED ALONG WITH TERMS FOR NON-BONDED INTERACTIONS AND TORSIONAL POTENTIAL ENERGY.

INVTRP

INVTRP IS A PROGRAM TO PREPARE MATRICES DESCRIBING SPACE-GROUP SYMMETRY FOR USE IN PROGRAM AVSORT. PROGRAM INVTRP ACCEPTS 3X3 MATRICES FOR REAL-SPACE SYMMETRY TRANSFORMATIONS, AND FORMS THEIR INVERSE TRANSPOSE FOR USE IN RECIPROCAL SPACE. THE PROGRAM PRODUCES A PUNCHED DECK OF 'BLOCK DATA SYMOPS' WHICH SPECIFIES THE INVERSE TRANSPOSE MATRICES. 'BLOCK DATA SYMOPS' MAY BE USED DIRECTLY IN PROGRAM AVSORT.

JIMDAP

PROGRAM JIMDAP IS THE BROOKHAVEN MODIFICATION OF FORDAP, THE FOURIER-SYNTHESIS PROGRAM BY A. ZALKIN. JIMDAP IS QUITE FLEXIBLE, AND PROVIDES FOR AUTOMATIC PEAK SEARCH AND PLOTTING OF CONTOURED MAPS. FOR COMPUTATION OF FOURIER, DIFFERENCE FOURIER OR ORDINARY PATTERSON SYNTHESES, JIMDAP READS A FILE PRODUCED BY THE STRUCTURE FACTOR LEAST-SQUARES PROGRAM FLINUS. FOR COMPUTATION OF SHARPENED OR ORIGIN-REMOVED PATTERSON SYNTHESES, JIMDAP READS A FILE PRODUCED BY

PROGRAM XDATA.

LEASTSQ

PROGRAM LEASTSQ IS THE BROOKHAVEN MODIFICATION OF THE MULTIPLE ISOMORPHOUS REPLACEMENT (MIR) PHASING PROGRAM BY M. ROSSMANN ET AL. LEASTSQ IS A LEAST-SQUARES PROGRAM TO REFINE HEAVY-ATOM PARAMETERS IN AN ISOMORPHOUS SERIES AND TO OPTIMIZE PHASES CALCULATED BY THE MIR METHOD. PROGRAM LEASTSQ INCLUDES THE EFFECTS OF ANOMALOUS DISPERSION AND ALLOWS FOR UP TO 10 ISOMORPHOUS DERIVATIVES.

LIST

LIST IS A PROGRAM TO PRODUCE A LIST OF STRUCTURE FACTOR DATA FOR PUBLICATION. THE PROGRAM READS A FILE PRODUCED BY THE STRUCTURE FACTOR LEAST-SQUARES PROGRAM FLINUS, AND PRODUCES A LISTING SUITABLE FOR REDUCTION TO FIT ON AN 8 1/2 X 11 INCH PAGE. A TOTAL OF 6800 REFLECTIONS CAN BE ACCOMODATED, WITH 2000 REFLECTIONS LISTED PER PAGE AFTER REDUCTION. A LISTING IN SINGLE-COLUMN FORM MAY ALSO BE PRODUCED.

MULTAN

MULTAN IS THE PACKAGE OF DIRECT METHODS PROGRAMS BY G. GERMAIN, P. MAIN, AND M. M. WOOLFSON. THE MULTAN PACKAGE CONSISTS OF EIGHT PROGRAMS:

NORMAL

PROGRAM NORMAL CALCULATES NORMALIZED STRUCTURE FACTORS (E'S).

MULTAN

PROGRAM MULTAN IS THE DIRECT-METHODS PHASING PROGRAM WHICH FORMS THE HEART OF THE PACKAGE. THE PROGRAM INCLUDES SIGMA TWO RELATIONSHIPS, PSI ZERO TEST, CONVERGENCE MAPPING, AND MULTI-SOLUTION WEIGHTED TANGENT REFINEMENT. PROGRAM MULTAN AUTOMATICALLY WILL CHOOSE ORIGIN AND ENANTIOMORPH-DEFINING REFLECTIONS, OR OPTIONALLY THESE MAY BE SUPPLIED BY THE USER. THE PROGRAM ASSIGNS ARBITRARY PHASES TO A NUMBER OF GENERAL REFLECTIONS, AND USES THESE IN A WEIGHTED TANGENT REFINEMENT PROCEDURE, TO GENERATE MULTIPLE SOLUTIONS FOR PHASES OF REFLECTIONS WITH LARGE E VALUES.

EXPAND FFT SEARCH DANFIG MFRP

THESE FIVE PROGRAMS TOGETHER ALLOW FOR GENERATION OF E-MAPS, AUTOMATIC PEAK SEARCHING, PLOTTING ON PAPER OF TRIAL STRUCTURES, AND RECOGNITION OF MOLECULAR FRAGMENTS.

SF

PROGRAM SF ALLOWS FOR CALCULATION OF PHASES FROM PARTIAL STRUCTURES, AND THESE PHASES MAY THEN BE REINTRODUCED AS STARTING PHASES IN MULTAN.

NANOVA

NANOVA IS A PROGRAM TO ANALYZE FOR CORRELATIONS BETWEEN ABS(FO-FC)/SIGMA(FO) AND FO, AND BETWEEN ABS(FO-FC)/SIGMA(FO) AND SIN(THETA)/LAMBDA. IT IS OFTEN USEFUL TO PERFORM SUCH AN ANALYSIS OF VARIANCE AFTER REFINEMENT OF A STRUCTURE, IN ORDER TO TEST THE APPROPRIATENESS OF THE WEIGHTING SCHEME, AND ALSO TO LOOK FOR DEFICIENCIES IN THE PARTICULAR MODEL UPON WHICH THE REFINEMENT IS BASED. PROGRAM NANOVA CALCULATES THE MEAN ABS(FO-FC)/SIGMA(FO) FOR INTERVALS OF FO AND SIN(THETA)/LAMBDA, AND GIVES F STATISTICS FOR USE IN TESTS FOR SIGNIFICANT CORRELATIONS.

ORTEP2

ORTEP2 IS THE OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM BY C. JOHNSON. PROGRAM ORTEP2 PRODUCES CALCOMP PLOTS (OPTIONALLY IN STEREO) OF CRYSTAL STRUCTURES, WITH ATOMS REPRESENTED AS THERMAL ELLIPSOIDS. PROGRAM ORTEP2 INCLUDES AUTOMATIC OVERLAP REMOVAL.

ORTRAN

ORTRAN IS THE OAK RIDGE RECIPROCAL SPACE FOURIER-TRANSFORM SEARCHING PROGRAM BY W. BUSING AND W. THIESSEN. PROGRAM ORTRAN WILL SEARCH THE RECIPROCAL SPACE OF THE NORMALIZED STRUCTURE FACTORS FOR THE FOURIER TRANSFORM OF A KNOWN MOLECULAR FRAGMENT. SEARCHES MAY BE CARRIED OUT FOR MORE THAN ONE ORIENTATION OF A MOLECULAR FRAGMENT, AND THESE ORIENTATIONS SAVED, THUS DEFINING THE ORIENTATION OF REPEATED STRUCTURAL UNITS.

POWPAT

POWPAT IS A PROGRAM BY E. PARTHE ET AL. FOR THE INTENSITY CALCULATION OF POWDER PATTERNS. PROGRAM POWPAT IS QUITE GENERAL, AND MAKES PROVISION FOR CALCULATION OF INTENSITIES FOR ALL SPACE GROUPS. THE PROGRAM INCLUDES LP CORRECTIONS FOR POWDER PATTERNS RECORDED WITH A MONOCHROMATOR (NORMAL GEOMETRY OR GUINIER-DE WOLFF FOCUSING CAMERA). NO PROVISION IS MADE FOR ABSORPTION CORRECTIONS.

PRJCTNC

PRJCTNC IS THE VERSION OF PROGRAM PRJCTN FOR THE CDC 7600 AND 6600, AND WILL PRODUCE CALCOMP LINE-DRAWINGS OF MOLECULES IN STEREO. AN INTERACTIVE VERSION OF PROGRAM PRJCTN FOR THE PDP11 DRAWS MOLECULAR AND CRYSTAL STRUCTURES ON THE VECTOR GENERAL DISPLAY (SEE P III-15). PROGRAM PRJCTN REQUIRES SIMPLE INPUT, AND WILL ACCEPT ATOMIC COORDINATE DATA IN X-RAY SYSTEM FORMAT OR FLINUS FORMAT. MAIN-CHAIN DRAWINGS OF PROTEINS CAN BE MADE DIRECTLY, BY READING ATOMIC COORDINATES FROM THE PROTEIN DATA BANK. PROGRAM PRJCTN WILL ACCOMODATE 97 ATOMS AND DRAW UP TO 200 BONDS.

PROCK

PROCK IS A PROGRAM FOR INTEGRATION OF PEAK PROFILES AND SUBTRACTION OF BACKGROUNDS. PROGRAM PROCK IS THE FIRST STAGE IN PROCESSING DECOLLATED DATA FROM THE DIFFRACTOMETERS RUNNING UNDER THE RECF SYSTEM. PROCK

PROVIDES A NUMBER OF PROFILE-INTEGRATION SCHEMES, INCLUDING USE OF THE "MINIMUM SIGMA(I)/I" METHOD OR A SMOOTHING ALGORITHM. THE OUTPUT OF PROGRAM PROCK, WHICH INCLUDES INTEGRATED INTENSITIES, BACKGROUNDS AND SETTING ANGLES CORRECTED FOR MECHANICAL ZEROES AND AXIS PARITIES, IS SUITABLE FOR USE AS INPUT TO PROGRAMS ABSOR, BNLABS, OR CORDAT.

SADIAN

SADIAN IS A PROGRAM WHICH CALCULATES INTER-ATOMIC DISTANCES AND ANGLES IN CRYSTAL STRUCTURES. PROGRAM SADIAN SEARCHES FOR ALL INTERATOMIC DISTANCES AND/OR BOND ANGLES WITHIN 26 UNIT CELLS SURROUNDING THE REFERENCE UNIT CELL, UP TO SPECIFIED LIMITS. THE PROGRAM HANDLES ANY SYMMETRY FROM TRICLINIC TO CUBIC. PROGRAM SADIAN CAN ACCOMODATE 200 ATOMS, 48 SYMMETRY OPERATIONS, AND EIGHT LATTICE TRANSLATIONS.

SANDA

SANDA IS A PROGRAM BY R. SHIONO FOR CALCULATION OF INTER-ATOMIC DISTANCES AND BOND ANGLES. PROGRAM SANDA PERFORMS FUNCTIONS SIMILAR TO THOSE PERFORMED BY PROGRAM SADIAN. SANDA WILL ACCOMODATE UP TO 175 ATOMS, AND 192 SYMMETRY OPERATIONS. A VERSION OF SANDA IS ALSO AVAILABLE FOR THE PDP11 (SEE P III-15).

SCAT

SCAT IS A PROGRAM TO PRODUCE X-RAY SCATTERING-FACTOR CARDS IN A FORMAT SUITABLE FOR USE IN THE STRUCTURE FACTOR LEAST-SQUARES PROGRAM FLINUS. PROGRAM SCAT CONTAINS THE COEFFICIENTS FOR 212 ATOMS AND IONS DISTRIBUTED BY D. CROMER FOR CALCULATION OF SCATTERING FACTORS BY THE METHOD OF D. CROMER AND J. MANN.

STRONG

STRONG IS A PROGRAM TO CALCULATE REFLECTIONS WITH STRONG NEUTRON INTENSITIES, FOR A KNOWN STRUCTURE. PROGRAM STRONG WILL LIST ALL UNIQUE REFLECTIONS APPROPRIATE TO THE USER'S CELL TYPE WHICH HAVE AN INTENSITY ON AN ABSOLUTE SCALE GREATER THAN 1.0. A SEPARATE LIST OF REFLECTIONS, WITHIN A SPECIFIED TWO THETA RANGE AND SORTED ON INTENSITY, IS PRODUCED FOR USE IN CONJUNCTION WITH THE RECF CRYSTAL-ORIENTATION PROGRAM ORIENT. PROGRAM STRONG WILL ALLOW UP TO 200 ATOMS PER UNIT CELL (ACENTRIC) OR UP TO 400 ATOMS PER UNIT CELL (CENTRIC STRUCTURES).

TLS6

TLS6 IS THE BROOKHAVEN MODIFICATION OF THE RIGID-BODY MOTION ANALYSIS PROGRAM BY V. SCHOMAKER AND K. TRUEBLOOD. THE PROGRAM CALCULATES THE BEST FIT TO OBSERVED THERMAL PARAMETERS FOR A GENERAL RIGID-BODY MOTION DESCRIBED IN TERMS OF TRANSLATION (T), LIBRATION (L), AND SCREW (S) TENSORS. INTERATOMIC DISTANCES ARE CORRECTED FOR EFFECTS OF THERMAL MOTION BASED UPON THE CALCULATED VALUES OF L.

TORSION

TORSION IS THE BROOKHAVEN MODIFICATION OF A PROGRAM FOR CALCULATION OF TORSION ANGLES BY G. L. GARTLAND AND R. SHIONO. TORSION ANGLES ARE

CALCULATED IN THE STANDARD IUPAC-IUB CONVENTION, WITH ZERO TORSION ANGLE CORRESPONDING TO THE CIS CONFORMATION. PROGRAM TORSION CAN ACCOMODATE UP TO 100 ATOMS.

TRACER

TRACER IS A CELL-REDUCTION PROGRAM BY S. LAWTON. PROGRAM TRACER PERFORMS A BUERGER REDUCTION, TO CALCULATE THE REDUCED UNIT CELL CORRESPONDING TO THE INPUT CELL PARAMETERS. PROGRAM TRACER EXAMINES THE NIGGLI MATRIX CORRESPONDING TO THE REDUCED CELL. SPECIAL RELATIONSHIPS ARE SOUGHT WHICH IMPLY CELL DIMENSIONS THAT CONFORM TO A PARTICULAR CRYSTAL CLASS.

VECTOR VECTR1

VECTOR IS A LIBRARY OF SUBROUTINES FOR HANDLING COMMON GEOMETRICAL AND CRYSTALLOGRAPHIC COMPUTATIONS IN 3-SPACE. THE FUNCTIONS PERFORMED INCLUDE VECTOR SUM, DIFFERENCE, AND ROTATION, ALIGNMENT OF TWO PAIRS OF VECTORS, MATRIX INVERSION AND TRANSPOSITION, AND CALCULATION OF ORTHOGONALIZATION MATRICES. PROGRAM VECTR1 IS A REVERSE-POLISH NOTATION KEYBOARD CALCULATOR ROUTINE. IT EMPLOYS THE LIBRARY VECTOR AND CAN BE USED TO TREAT SCALARS, 3-SPACE VECTORS, AND 3X3 MATRICES. SEPARATE REGISTER STACKS ARE AVAILABLE FOR SCALARS, VECTORS, AND MATRICES, AND ONE MEMORY SLOT IS AVAILABLE FOR EACH. SCALAR-SCALAR, VECTOR-VECTOR, MATRIX-VECTOR, AND MATRIX-MATRIX MULTIPLICATION ARE SOME TYPICAL OPERATIONS THAT CAN BE PERFORMED. A VERSION OF VECTOR IS ALSO AVAILABLE FOR THE PDP11 (SEE P. III-13).

XDATA

XDATA IS A PROGRAM TO CALCULATE SCALE FACTORS AND OVERALL TEMPERATURE FACTORS FROM WILSON PLOTS. PROGRAM XDATA PRODUCES SCALED STRUCTURE FACTOR DATA SUITABLE FOR INPUT TO THE STRUCTURE FACTOR LEAST-SQUARES PROGRAM FLINUS. XDATA ALSO PRODUCES DATA SUITABLE FOR INPUT TO THE FOURIER SYNTHESIS PROGRAM JIMDAP FOR THE CALCULATION EITHER OF ORDINARY PATTERSON SYNTHESIS, SHARPENED PATTERSON, OR SHARPENED PATTERSON WITH ORIGIN REMOVED.

4. PROTEIN DATA BANK

THE PROTEIN DATA BANK IS A COMPUTER-BASED LIBRARY OF STRUCTURAL DATA, WHICH SERVES AS AN ARCHIVAL STORAGE MEDIUM FOR STRUCTURE FACTORS, PHASES AND ATOMIC COORDINATES FOR MACROMOLECULES. THE DATA BANK IS MAINTAINED AT BROOKHAVEN ON A CDC UPDATE PROGRAM LIBRARY, AND CAN BE ACCESSED VIA THE CRYSNET TERMINALS. A COPY OF THE FILE IS KEPT IN CAMBRIDGE, ENGLAND AT THE CRYSTALLOGRAPHIC DATA CENTRE. THE DATA BANK DISTRIBUTES DATA UPON REQUEST ON MAGNETIC TAPE; BROOKHAVEN HANDLES DISTRIBUTION WITHIN THE U.S. AND CANADA, AND CAMBRIDGE OUTSIDE NORTH AMERICA.

THE FORMAT OF ATOMIC COORDINATE DATA IN THE BANK IS DESCRIBED IN DETAIL IN APPENDIX 3. EXTENSIVE DESCRIPTIVE INFORMATION IS INCLUDED AT THE HEAD OF THE FILE FOR EACH PROTEIN. ATOMIC COORDINATE RECORDS ARE EACH 132 CHARACTERS; THEIR FORMAT IS A MODIFICATION OF THAT EMPLOYED IN THE REAL-SPACE REFINEMENT PROGRAM OF R. DIAMOND. PROGRAM PROIN IS USED TO PROCESS CONTRIBUTED DATA INTO THE STANDARD FORMAT. DOCUMENTATION FOR PROGRAM PROIN IS INCLUDED IN APPENDIX 2.

A PROGRAM SEARCH IS AVAILABLE TO RETRIEVE ATOMIC COORDINATE DATA FROM THE BANK. THESE DATA MAY THEN BE USED AT THE CRYSNET TERMINALS, FOR EXAMPLE TO DISPLAY STRUCTURAL FEATURES ON THE VECTOR GENERAL CRT WITH PROGRAM PRJCTN (SEE P. III-15). WITH PROGRAM SEARCH, IT IS POSSIBLE TO EXTRACT ATOMIC COORDINATES FOR ALL ATOMS WITHIN A SPECIFIED RADIUS OF A TARGET ATOM (OR GROUP OF ATOMS) IN A PARTICULAR PROTEIN. SEARCHES MAY BE SELECTIVE, E.G. TO EXTRACT ONLY ALPHA-CARBON ATOMS, ETC. TO EXECUTE PROGRAM SEARCH ON THE CDC 7600, FOLLOW THE SAMPLE JOB SET-UP GIVEN BELOW:

```
1.  JOB03,CP70,YD1,EC64,T77,TP0.      SAMPLE 7600 SEARCH
2.  ACCOUNT,MURPHY,899.
3.  MOUNT,VSN=ISTRY1,SN=ISTRY.
4.  ATTACH,BUPD140,ID=CPROGS,SN=ISTRY.
5.  ATTACH,OLDPL,PDBPL,ID=PDB,SN=ISTRY.
6.  BUPD140,Q,D,8,C=TAPE1.
7.  RETURN,OLDPL.
8.  ATTACH,SEARCH,ID=PDB,SN=ISTRY.
9.  FILE,TAPE12,RT=Z,BT=C,FL=80.
10. REQUEST,TAPE12,*PF.
11. SEARCH.
12. REWIND,TAPE12.
13. CATALOG,TAPE12,SEARCHOUTPUTFORPRJCTN,RP=7,
....ID=MURPHY,XR=MURPHY,AC=899,ST=MFA.
14. REWIND,TAPE12.
15. COPYSBF,TAPE12,OUTPUT.
16. 7/8/9
17. *COMPILE,THERM001
18. 7/8/9
....12345678901234567890123456789 0
19.     1    1  999.              2
20.   -99
21. END-OF-FILE
```

NOTES

4. BUPD140 IS A VERSION OF CDC UPDATE FOR 140-CHARACTER LINES.

5. ATTACH THE PROTEIN DATA BANK PROGRAM LIBRARY. THE FILE PDBPL IS STORED ON SN=ISTRY, BUT DUE TO SPACE LIMITATIONS IS NOT KEPT ON SN=CHEM. DECKS CONTAINING STRUCTURE FACTORS AND PHASES ARE NOT KEPT ON THE FILE PDBPL. THESE DECKS EXIST ON A PROGRAM LIBRARY WHICH MAY BE STAGED IN FROM MAGNETIC TAPE C495 (SEVEN-TRACK, 556 BPI, LABELLED TAPE, RT=S).

6. WRITE THE FILE FOR A PARTICULAR PROTEIN ON TAPE1.

9. THIS FILE STATEMENT SPECIFIES THE SCOPE 3.4 (6600) DEFAULT FORMAT FOR CODED FILE.

13. CATALOG TAPE12, WHICH CONTAINS ATOMIC COORDINATES IN A FORMAT SUITABLE FOR INPUT TO PROGRAM PRJCTN. TAPE12 IS CATALOGED ON THE 6600, FOR EASY ACCESS VIA INTERCOM.

15. THIS CARD SHOULD BE REPEATED ONCE FOR EACH SEARCHING OPERATION CARRIED OUT. TAPE12 WILL CONTAIN ONE FILE FOR EACH OPERATION.

17. THERMO01 IS THE DECKNAME ON PDBPL FOR THERMOLYSIN. TABLE IV-2 GIVES A COMPLETE LIST OF DECK NAMES FOR PROTEINS CURRENTLY ON FILE.

19. THIS CARD WILL EXTRACT ALL ALPHA CARBON ATOMS IN A PROTEIN. FOR DETAILS CONCERNING OTHER POSSIBLE TYPES OF SEARCHES, SEE THE PROGRAM DOCUMENTATION IN APPENDIX 2.

20. TERMINATOR

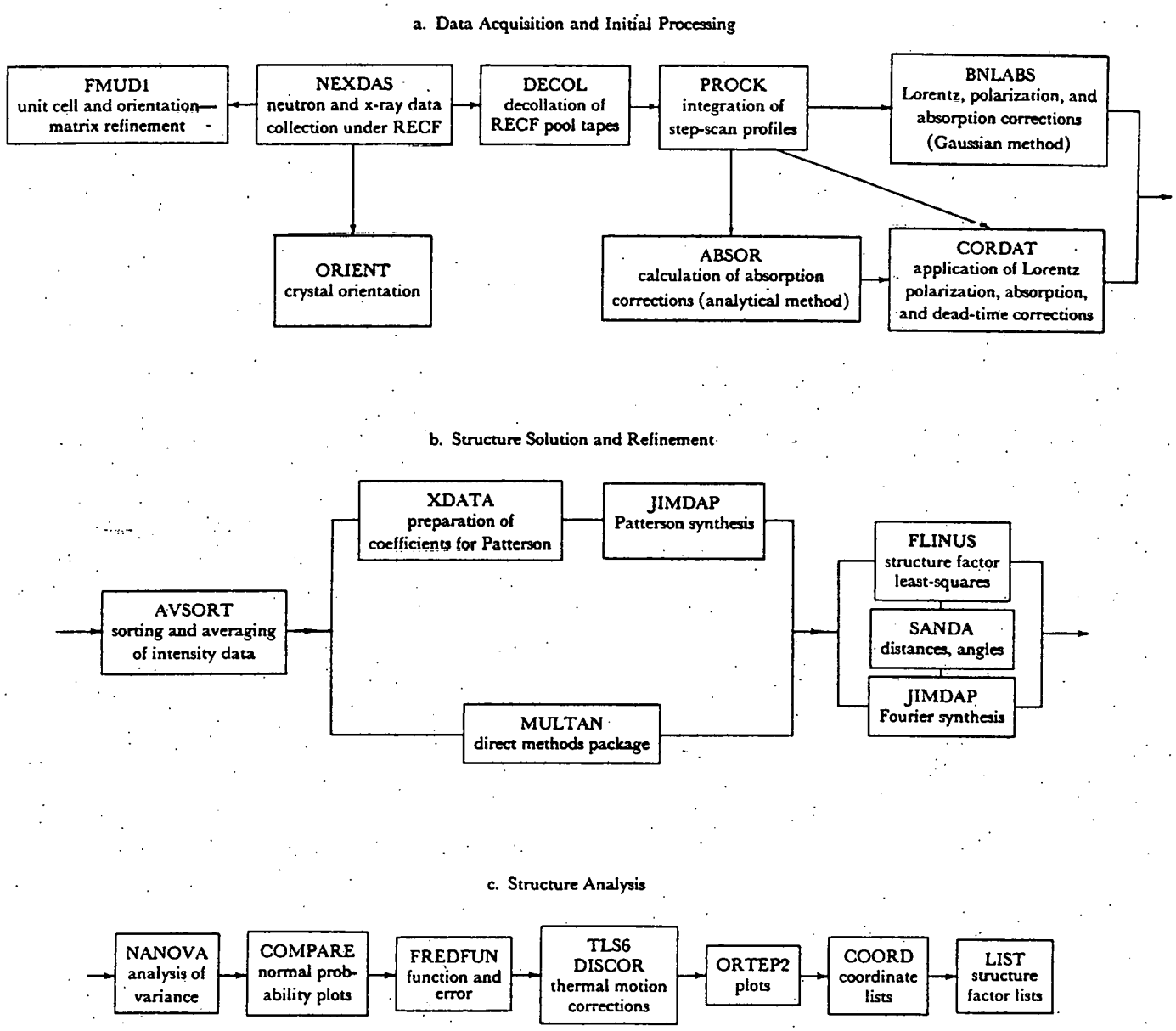

FIGURE IV-1. General Flow of Brookhaven Crystallographic Computer Programs.

FIGURE IV-1

TABLE IV-1. BROOKHAVEN LIBRARY OF CRYSTALLOGRAPHIC PROGRAMS FOR USE ON CDC 7600 AND 6600.

PROGRAM	PURPOSE
ABSOR	CALCULATE ABSORPTION CORRECTIONS (ANALYTICAL METHOD)
ACCESS	FILE RETRIEVAL UTILITY
AVBANG	CALCULATE MEANS AND VARIANCES (DISTANCES AND ANGLES)
AVSORT	SORT AND AVERAGE EQUIVALENT REFLECTION DATA
BNLABS	ABSORPTION AND LP CORRECTIONS (GAUSSIAN INTEGRATION)
COMPARE	CARRY OUT STATISTICAL COMPARISONS OF EXPERIMENTAL RESULTS
COORD	PRODUCE PUBLISHABLE LISTINGS OF ATOMIC PARAMETERS
CORDAT	APPLY CORRECTION FACTORS TO F**2 AND SIG(F**2)
DECOL	DECOLLATE RECF POOL TAPES
DISCOR	CORRECT BOND DISTANCES FOR THERMAL MOTION
EDIT	CONTEXT EDITOR UTILITY
EFACTH	CALCULATION OF NORMALIZED STRUCTURE FACTORS
EXAMOR	PROCESS ORACLE TAPES FOR PROCK
FACES	DETERMINE CRYSTAL BOUNDARY PLANES
FLINUS	FULL-MATRIX LEAST-SQUARES REFINEMENT
FMUD1	LEAST-SQUARES REFINEMENT OF CELL CONSTANTS AND ANGLES
FREDFUN	CRYSTALLOGRAPHIC FUNCTIONS AND ERRORS (WITH CORRELATIONS)
GENATM	GENERATION OF NEW ATOMIC POSITIONS WITH GEOM. CONSTRAINTS
HERM	MODEL BUILDING AND ENERGY MINIMIZATION OF PROTEINS
INRSCL	INTERLAYER SCALING OF X-RAY PHOTOGRAPHS
INVTRP	PREPARE SYMMETRY MATRICES FOR AVSORT
JIMDAP	FOURIER SYNTHESIS
LEASTSQ	MULTIPLE ISOMORPHOUS REPLACEMENT PHASING PROGRAM
LIST	PREPARES LIST OF REFLECTION DATA FOR PUBLICATION
MULTAN	DIRECT METHODS PACKAGE (EIGHT PROGRAMS)
NANOVA	CORRELATIONS OF DELTA/SIG AND FOBS, DELTA/SIG AND SINT/L
OMULT	EARLIER VERSION OF MULTAN (ONE PROGRAM ONLY)
ORTEP2	THERMAL ELLIPSOID PLOTTING PROGRAM
ORTRAN	RECIPROCAL SPACE FOURIER-TRANSFORM SEARCH
POWPAT	INTENSITY CALCULATION OF POWDER PATTERNS
PRJCTNC	PRODUCE LINE DRAWINGS OF MOLECULES ON CALCOMP PLOTTER
PROCK	INTEGRATION OF PEAK PROFILES AND SUBTRACTION OF BACKGRND
PROIN	PREPARE DATA FOR PROTEIN DATA BANK
RMCOPY	COPY UTILITY USING RECORD MANAGER
SADIAN	SEARCH FOR INTER-ATOMIC DISTANCES AND ANGLES
SANDA	CALCULATE DISTANCES AND ANGLES
SCAT	PREPARE X-RAY SCATTERING FACTORS FOR FLINUS
SEARCH	RETRIEVE COORDINATES FROM PROTEIN DATA FILES
STRONG	CALULATE REFLECTIONS WITH STRONG NEUTRON INTENSITIES
TLS6	RIGID-BODY MOTION ANALYSIS (SCHOMAKER-TRUEBLOOD METHOD)
TORSION	CALCULATE TORSION ANGLES
TRACER	CELL REDUCTION (BUERGERS METHOD)
TYPIST	UTILITY DOCUMENTATION PROGRAM
VECTOR	LIBRARY OF THREE-DIMENSIONAL LINEAR-ALGEBRA ROUTINES
VECTR1	CALCULATOR PROGRAM FOR SCALARS, VECTORS, AND MATRICES
XDATA	OBTAIN SCALE AND TEMPERATURE FACTORS FROM WILSON PLOTS

TABLE IV-2.

PROTEIN DATA BANK: DECK NAMES FOR PROTEINS CURRENTLY ON FILE

DECK	PROTEIN	CONTRIBUTOR	CONTENTS*
CHYMO1	TOSYL ALPHA-CHYMOTRYPSIN	D. M. BLOW	AC
CHYMO2	TOSYL ALPHA-CHYMOTRYPSIN	D. M. BLOW	AC
CHYMOF	TOSYL APLPHA-CHYMOTRYPSIN	D. M. BLOW	SF
CMPF6A01	MYOGEN (REFINED SET F6A)	R. H. KRETSINGER	AC
CMPF6H01	MYOGEN (REFINED SET F6H)	R. H. KRETSINGER	AC
CMPF6I01	MYOGEN (REFINED SET F6I)	R. H. KRETSINGER	AC
CONCNA01	CONCANAVALIN A	K. D. HARDMAN	AC
CONCNA02	CONCANAVALIN A	G. M. EDELMAN	AC TA
CPASE01	CARBOXYPEPTIDASE A	W. N. LIPSCOMB	AC
CTPSGN01	CHYMOTRYPSINOGEN	J. KRAUT	AC
CYTB501	CYTOCHROME B5	F. S. MATHEWS	AC
CYTB502	CYTOCHROME B5	F. S. MATHEWS	TA
CYTOC201	CYTOCHROME C2	J. KRAUT	AC
DISMUT01	SUPEROXIDE DISMUTASE(ALPHA-C)	D. AND J. RICHARDSON	AC
FLVDXN01	FLAVODOXIN	M. L. LUDWIG	AC TA
HDOXHB01	DEOXY-HEMOGLOBIN (HUMAN)	M. F. PERUTZ	AC TA
HIPIPR01	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	AC
HSDEHB01	DEOXY-HEMOGLOBIN (HORSE)	M. F. PERUTZ	AC TA
HSMEHB01	MET-HEMOGLOBIN (HORSE)	M. F. PERUTZ	AC TA
LAMP1	HEMOGLOBIN (SEA LAMPREY)	W. A HENDRICKSON W. E. LOVE	AC TA
LAMPREY0	HEMOGLOBIN (SEA LAMPREY)	W. A. HENDRICKSON W. E. LOVE	SF
LDH01	LACTATE DEHYDROGENASE (APO) (UNREFINED SET)	M. G. ROSSMANN	AC TA
LDH02	LACTATE DEHYDROGENASE (APO) (REFINED SET)	M. G. ROSSMANN	AC TA
LOBGPD01	D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (GREEN SUBUNIT)	M. G. ROSSMANN	AC TA
LOBGPD02	D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (RED SUBUNIT)	M. G. ROSSMANN	AC TA
LYHOH001	LYSOZYME (SOLVENT MOLECULES)	R. DIAMOND	AC TA
LYRS5D01	LYSOZYME (REFINED SET RS5D)	R. DIAMOND	AC TA
LYRS6A01	LYSOZYME (REFINED SET RS6A)	R. DIAMOND	AC TA
LYRS9A01	LYSOZYME (REFINED SET RS9A)	R. DIAMOND	AC TA
LYRS12A1	LYSOZYME (REFINED SET RS12A)	R. DIAMOND	AC TA
LYRS1601	LYSOZYME (REFINED SET RS16)	R. DIAMOND	AC TA
LYSOW201	LYSOZYME (REFINED SET W2)	R. DIAMOND	AC TA
MYOGL01	MYOGLOBIN	J. C. KENDREW H. C. WATSON	AC
PAPAIN01	PAPAIN	J. DRENTH	AC TA
RCARP04	MYOGEN	R. H. KRETSINGER	SF
RCARP05	MYOGEN (HEAVY ATOM DATA)	R. H. KRETSINGER	SF
RHUMDEH02	DEOXY-HEMOGLOBIN (HUMAN)	M. F. PERUTZ	SF

* AC = ATOMIC COORDINATES, TA = TORSION ANGLES, SF = STRUCTURE FACTORS AND PHASES.

DECK	PROTEIN	CONTRIBUTOR	CONTENTS*
RNASES01	RIBONUCLEASE S	F. M. RICHARDS	AC
RUBY01	RUBREDOXIN (UNREFINED SET)	H. W. WYCKOFF L. H. JENSEN	AC
RUDOXN02	RUBREDOXIN	L. H. JENSEN	AC
STAPHN01	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON	AC
SUBTLE1	SUBTILISIN BPN'	E. E. HAZEN J. KRAUT	AC
TERNRY01	LDH NAD PYRUVATE COMPLEX	M. G. ROSSMANN	AC TA
THERMO01	THERMOLYSIN (UNREFINED SET)	B. W. MATTHEWS	AC
THERMO02	THERMOLYSIN (REFINED SET)	B. W. MATTHEWS	AC
TORSNA01	TORSION ANGLES (11 PROTEINS)	E. A. KABAT	TA
TRIN01	PANCREATIC TRYPSIN INHIBITOR	T. T. WU R. HUBER	AC
TRIN02	PANCREATIC TRYPSIN INHIBITOR	R. HUBER	AC TA

* AC = ATOMIC COORDINATES, TA = TORSION ANGLES, SF = STRUCTURE FACTORS AND PHASES.

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APPENDIX 1. TERMINAL PROGRAM WRITEUPS

AMD - CDC 200 UT SIMULATOR
CRYSNET UTILITY PROGRAM RELEASE
HERBERT J. BERNSTEIN

SOFTWARE DEVELOPED UNDER CONTRACT NO. AG-370
WITH THE NATIONAL SCIENCE FOUNDATION AT

BROOKHAVEN NATIONAL LABORATORY
DEPARTMENT OF CHEMISTRY
UPTON, L.I., NEW YORK 11973

UNDER THE AUSPICES OF ERDA.

DIRECT INQUIRIES TO ***** CRYSNET PROJECT ******

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THIS TAPE CONTAINS THE MATERIALS NEEDED TO INTRODUCE A SIMULATOR FOR A CDC 200 SERIES USER TERMINAL IN DOS V08-08 OR V09-19, ASSUMING ONE HAS A DEC DP11 SYNCHRONOUS INTERFACE AND BELL 201A COMPATIBLE MODEM ON A DEC PDP11 WITH AT LEAST 16K OF CORE. A DRIVER FOR A DU11 IS ALSO INCLUDED, BUT IS NOT YET FULLY TESTED.

THE CODE WAS WRITTEN BY G.H.CAMPBELL, AND H.B. CHIANG OF BROOKHAVEN NATIONAL LABORATORY, USING THE UTEX "TWOSIM" PACKAGE AS A MODEL (UTEX-CC-TPB-133, THE UNIVERSITY OF TEXAS AT AUSTIN, OCTOBER 1973), MODIFIED BY T. V. WILLOUGHBY OF THE UNIVERSITY OF LEEDS, AND EXTENSIVELY REVISED BY H.J. BERNSTEIN OF BNL. A SERIOUS ATTEMPT HAS BEEN MADE NOT TO VIOLATE CONTROL DATA CORPORATION SYSTEM STANDARD 1.10.020 TOO SERIOUSLY, AND STILL HAVE THE CODE WORK.

ONE NEEDS THE STANDARD DEC RELEASE MATERIALS FOR DOS OR BATCH SINCE THE CIL MUST BE RECONFIGURED TO INCLUDE A NEW DRIVER (DV.MR) AND THE DRIVER DV.KB MUST BE REPLACED. TO GET NOTICE OF UPDATES, PLEASE REGISTER WITH:

HERBERT J. BERNSTEIN
CHEMISTRY DEPARTMENT
BROOKHAVEN NATIONAL LABORAORY
UPTON, L.I., NEW YORK 11973
PHONE (516) 345 4378

THIS IS THE THIRD RELEASE OF THIS PACKAGE, AND THE SECOND TO BE DEPOSITED IN THE DECUS LIBRARY. THIS VERSION OBSOLETES THE PRIOR VERSIONS (08-JUN-74, AND 10-MAY-74), CORRECTING MOST KNOWN BUGS, AND INTRODUCING SEVERAL NEW FEATURES. IN PARTICULAR, THE CODE NOW SUPPORTS BOTH ANSI AND BCD 200 UT PROTOCOLS, AND WORKS AGAINST CDC INTERCOM VERSION 4.2, AS WELL AS SEVERAL NON-STANDARD CENTRAL SITE PROTOCOLS. COMMAND STRING SWITCH LOGIC HAS BEEN OVERHAULED, AND SWITCHES ARE NOW AVAILABLE TO SPECIFY SITE ADDRESS, TRANSMISSION CODE, CARRIAGE CONTROL, END-RECORD CHARACTER, ETC. ON INPUT, TAB CHARACTERS (CONTROL-I) ARE CONVERTED TO 1-8 BLANKS TO MATCH STANDARD DEC KB OUTPUT FORMATTING.

THE DRIVER HAS BEEN MODIFIED TO ALLOW FOR OTHER DEVICES GOING NOT READY BY TRANSMITTING AN IDLE MESSAGE. THIS SHOULD AVOID A MAJOR CAUSE OF DISCONNECTS.

THE PROGRAM IS NOW BEING MAINTAINED IN CDC UPDATE FORMAT, AS FURTHER CORRECTIONS, AND ADDITIONS ARE MADE, THEY WILL BE MADE AGAINST THE SEQUENCE NUMBERS ON THE RIGHT OF THE LISTINGS. FUTURE REVISIONS ARE ANTICIPATED.

IF YOU HAVE A PRIOR RELEASE OF THIS PACKAGE, BE SURE TO REPLACE THE DRIVER FOR THE MODEM (DP.MAC OR DU.MAC) AS WELL AS AMD, SINCE OLD VERSIONS OF THE DRIVER WILL NOT HANDLE THE CHANGED SPECIAL FUNCTIONS, AND THE NEW AMD WITH OLD DRIVERS WILL CLOBBER LOW CORE.

THE KNOWN DEFICIENCIES IN THIS VERSION ARE AS FOLLOWS:

DIAGNOSTIC WRITE IS NOT SUPPORTED. CODE FOR THIS MESSAGE TYPE IS AVAILABLE AND WILL BE INCLUDED WHEN A CENTRAL SITE IS FOUND THAT SUPPORTS THIS MESSAGE.

THE PROGRAM CANNOT BE USED IN BATCH MODE. NO SOLUTION IS YET AVAILABLE.

THE PROGRAM CANNOT BE RELIABLY TERMINATED BY TWO CONTROL-D COMMANDS IF THE CENTRAL SITE STOPS POLLING. THUS, TO ENSURE PROPER TERMINATION OF OUTPUT DATA SETS, THE USER SHOULD EXPLICITLY TERMINATE THEM BEFORE TERMINATING THE PROGRAM.

IN SOME CASES, THE KEYBOARD OUTPUT LOGIC OF THE SIMULATOR APPEARS TO FAIL TO START A NEW LINE AT THE SAME POINT THAT A REAL 200 UT DOES. THIS HAS APPEARED AS A CHARACTER INTENDED FOR COLUMN 1 PRINTING IN COLUMN 80. NO CHARACTERS ARE LOST, AND POSITION IS USUALLY RECOVERED WITH THE NEXT LINE. THE CAUSE IS NOT YET KNOWN.

WHEN RUNNING THE SIMULATOR, THE USE OF CONTROL-C, PR TO TERMINATE A PRINT OUT ON A TTY MAY CAUSE THE TTY TO CHATTER WITH A STRING OF NULLS. A SECOND CONTROL-C FOLLOWED BY A CARRIAGE RETURN APPEARS TO STOP THE THE CHATTER. THE PROBLEM APPEARS TO BE DUE TO THE PENDING KEYBOARD INPUT OF THE PROGRAM. RESOLUTION IN THE KEYBOARD DRIVER IS PLANNED.

THE FILES ON THIS TAPE ARE:

```
AMD.DOC          - THIS NOTE.
FEATSW.MAC       - DOS V08-08 DEC STANDARD FEATURES SWITCHES
                   USE THE V9-19 VERSION FROM RELEASE MATERIALS
                   FOR THAT SYSTEM.
PRAMTR.MAC       - NECESSARY DEFINITIONS FOR KB.MAC, ETC.,
                   FOR V08-08.  USE COPY FROM RELEASE MATERIALS
                   IF UNDER V9-19.
MATCHR.MAC       - A LITTLE ROUTINE WHICH MUST BE LINKED WITH
                   THE KEYBOARD DRIVER.
AMD.MAC          -THE PROGRAM WHICH SIMULATES A 200 UT.
DP.MAC           - DOS DRIVER FOR DP11
DU.MAC           - DOS DRIVER FOR DU11 (PRELIMINARY)
KB.MAC           - EXTENSIVELY REVISED KEYBOARD DRIVER.  THE
                   ESSENTIAL FEATURE USED IS THAT WHEN KB INPUT
                   IS PENDING, WRITES TO KB STILL GO THROUGH.  AS A
                   LITTLE BONUS, THE DRIVER WILL READ BINARY PAPER
                   TAPES FROM DEVICE PT:.
                   *** WARNING UNLESS YOU CHANGE THE SYMBOL
                   KBQUCH IN KB.MAC, WHEN YOU RUN WITH THIS
                   DRIVER, AN * WILL APPEAR WHENEVER THE DRIVER
                   WANTS INPUT.***
                   *** ALSO CONTROL-D CAUSES AN EOM STATUS
                   AND WILL TERMINATE MOST UTILITIES.***
SYSTEM.MAC       - TYPICAL RECONFIGURED V08-08.
                   NOTE, OUR DP11 IS AT INTERRUPT VECTOR 300,
                   YOURS MAY BE ELSEWHRE, IN WHICH CASE, CONFIGURE
                   HERE AND CHANGE THE DEFINITIONS IN MR.MAC.
AMD.OBJ,MATCHR.OBJ,KB.OBJ,DP.OBJ,DU.OBJ - OBJ'S.
".LST            - LISTINGS OF ASSEMBLIES.
KB.LDA,DP.LDA,DU.LDA - DRIVERS USING V08-08 DEFINITIONS
AMD.LDA          - 16K VERSION OF AMD.
".MAP            - LOAD MAPS.
DOSMTR.LCL       - A V08-08 SYSTEM WITH THESE AND OTHER DRIVERS IN.
TAPE.DIR         - CHECKSUMMED DIRECTORY OF THIS TAPE
```

JUST FOLLOW THE DIRECTIONS IN THE SYSTEM MANAGERS GUIDE, AND YOU SHOULD GET THIS IN WITH NO TROUBLE. IF NOT, PLEASE CALL. ONCE YOU HAVE THE DRIVERS IN, AND AMD.LDA IN UNDER 1,1, THEN YOU CAN RUN AMD. YOU WILL GET A LINE GIVING THE NAME AMD, AND THE DATE 22-JAN-75, FOLLOWED BY A LINE WITH A #. ANSWER WITH A DOS COMMAND STRING. THE FIRST TIME, TYPE /HE FOR A LIST OF SWITCHES ALLOWED. YOU DO NOT HAVE TO SPECIFY THE DATA SET PLAYING THE ROLE OF LINE PRINTER UNTIL YOU ACTUALLY HAVE SOMETHING TO PRINT. FOR MANY CENTRAL SITES, YOU MUST SPECIFY THE SITE ADDRESS WITH THE /SI SWITCH TO IDENTIFY THE TERMINAL TYPE (E.G. /SI:161 FOR AN ANSI 200 UT AGAINST CDC INTERCOM VERSION 4.2, OR /SI:160 FOR A BCD 200 UT).

GOOD LUCK.

AMD - CDC 200 UT SIMULATOR
CRYSNET UTILITY PROGRAM OPERATING INSTRUCTIONS

THIS NOTE IS INTENDED TO PROVIDE INSTRUCTIONS ON HOW TO RUN THE 200 UT SIMULATOR, BUT NOT BE SO SPECIFIC AS TO LIMIT COMMENTS TO A PARTICULAR CENTRAL SITE. THE SIMULATOR IS CODE WHICH ALLOWS A PDP-11 RUNNING UNDER DOS TO ACT AS A STANDARD CONTROL DATA CORPORATION REMOTE BATCH/INTERACTIVE TERMINAL FOR 2000 BAUD COMMUNICATIONS VIA DIAL-UP TELEPHONE LINES. THIS SIMULATOR WILL TALK TO CENTRAL SITES DEMANDING ANSI OR BCD PROTOCOLS. YOU NEED NOT KNOW WHAT THE CENTRAL SITE REQUIRES PROVIDED THE CENTRAL SITE TRANSMITS AT LEAST ONE MESSAGE BEFORE THE TERMINAL HAS TO.

IN ORDER TO RUN THE PROGRAM ONE MUST HAVE BOOTED IN DOS AND LOGGED IN UNDER A VALID UIC. THEN

```
RUN AMD
```

TO LOAD THE PROGRAM. THE PROGRAM WILL THEN TYPE OUT

```
AMD 22-JAN-75
#*
```

AND WAIT FOR A COMMAND STRING. THE PROPER REPLY DEPENDS ON THE PARTICULAR CENTRAL SITE. ONE DOES NOT HAVE TO PROVIDE ANY DATA SET SPECIFICATIONS AT THIS TIME, BUT ONE MAY HAVE TO SPECIFY THE PROPER SITE ADDRESS, AND POSSIBLY THE CODE SET (SEE SWITCHES BELOW). THESE ONLY HAVE TO BE GIVEN ONCE, NOT ON EVERY COMMAND STRING. IF YOU ARE PLANNING ORDINARY REMOTE BATCH AS AN EXTERNAL BCD TERMINAL WITH CARD READER AND LINE PRINTER, THE PROPER CCOMMAND STRING IS

```
LP:/SI:160/CO:E<CR:
```

WHILE IF YOU ARE NOT READY TO SPECIFY PARTICULAR DEVICES, AND WANT TO FOLLOW, SAY, INTERCOM VERSION 4.2, CONVENTIONS FOR AN ASCII TERMINAL, THE PROPER COMMAND STRING IS

```
/SI:161
```

LATER YOU COULD SPECIFY THE LINE PRINTER AND CARD READER BY TYPING CONTROL-D TO RETURN TO COMMAND MODE, AND THEN TYPING

```
LP:<CR:
```

IF YOU HAVE FILES ON DISK TO TRANSMIT, THEY WOULD REPLACE THE CR:, IF YOU WISH TO WRITE YOUR OUTPUT,SAY, ON MAGTAPE, THAT WOULD REPLACE LP:. ONLY ONE OUTPUT DATASET IS ALLOWED, BUT AS MANY INPUT DATASETS AS WILL FIT ON ONE LINE ARE ALLOWED. (A MODEM LOG OUTPUT DATA SET IS ALLOWED FOR DEBUGGING PURPOSES.) THE ARE MANY SWITCH OPTIONS AVAILABLE, WHICH WILL BE DESCRIBED BELOW. FIRST WE WILL RUN THROUGH THE COMMON CASE OF USING A LINE PRINTER AND CARD READER.

ONCE YOU HAVE TYPED THE FIRST COMMAND STRING, YOU MAY DIAL THE CENTRAL SITE. AS SOON AS THE CENTRAL SITE ANSWERS SWITCH TO DATA MODE, E.G. PULL UP THE WHITE BUTTON ON MANY TELEPHONES. THE PROGRAM SHOULD NOW

PRINT SOME CENTRAL SITE MESSAGE TO INDICATE CONNECTION. NOW THE KEYBOARD OF THE CONSOLE SHOULD BE LIVE TO THE CENTRAL SITE.

FOR SOME CENTRAL SITES, THE CONSOLE WILL BE TREATED EXACTLY AS IF IT WERE A DISPLAY, AND WILL ATTEMPT TO PERIODICALLY REFRESH, SAY, QUEUE DISPLAYS. THE PROGRAM IS TRAPPED TO NOT OUTPUT IDENTICAL SCREEN IMAGES. WHEN ANY LINE IS TYPED AT THE CONSOLE A LAST REPEAT OF SUCH A SCREEN MAY PRINT. SOME CENTRAL SITES ALSO PAUSE WHEN THEY BELIEVE A FULL SCREEN LOAD HAS BEEN TRANSMITTED, AND CONSIDER THE NEXT LINE INPUT ONLY AS A PERMISSION TO DISPLAY THE NEXT LOAD.

WHEN READING IN CARD DECKS, AN END-OF-RECORD IN 026 MODE IS A 7-8-9, AS FOR CDC 200-UTIS, BUT IN 029 MODE, THE END-OF-RECORD MUST BE AN 8-3 PUNCH. IN EITHER CASE, A # SIGN IS TREATED AS AN EOR. AN END OF FILE MAY BE PUNCHED BY PUTTING 17 IN COLUMNS 2 AND OF AN END-OF-RECORD CARD. THE CDC END-OF-FILE CARD 6-7-8-9 IS NOT RECOGNIZED. AN END OF FILE WILL ALSO BE TRANSMITTED ON READING A STANDARD DEC EOF (12-11-0-1-6-7-8-9) CARD PAIR.

IF THIS IS A NORMAL INSTALLATION OF THIS PACKAGE, THE SYSTEM WILL PRINT AN * WHENEVER INPUT FROM THE KEYBOARD OF THE CONSOLE CAN BE ACCEPTED. IF OUTPUT INTERRUPTS YOUR INPUT, THE INPUT ACCEPTED THUS FAR WILL BE REECHOED.

WHEN YOU WISH TO SIGN OFF, BE SURE TO SIGN OFF FROM THE CENTRAL SITE, THEN TYPE CONTROL-D FOLLOWED BY KB:<CR> TO CLOSE YOUR FINAL OUTPUT DATASET. THEN TERMINATE BY HANGING UP THE TELEPHONE AND KILLING THE PROGRAM.

NOW LET US CONSIDER THE GENERAL CASE. THE COMMAND STRINGS FOR THIS PROGRAM ARE OF THE FORM:

PRINT DATA SET, LOG DATA SET < CARD READER DATA SETS

WHERE THE PRINT DATA SET IS WRITTEN WITH ALL INFORMATION DIRECTED BY THE CENTRAL SITE TO A PRINTER, THE LOG DATA SET IS WRITTEN WITH FORMATTED BINARY RECOPDS CONSISTING OF THE NON-TRIVIAL MESSAGES TRANSMITTED FROM THE TERMINAL TO THE CENTRAL SITE, AND THE CARD READER DATA SETS ARE READ IN TURN AS IF THEY WERE THE TERMINAL CARD READER. IF THE PRINT DATA SET IS NOT SPECIFIED, THEN WHEN THE CENTRAL SITE ATTEMPTS TO TRANSMIT LINE TO THE PRINTER, THE MESSAGE

```
*** PRINT FILE REQUIRED ***
INPUT CONTROL-D AND COMMAND STRING
```

WILL APPEAR. AT THAT TIME A COMMAND STRING WITH A VALID PRINT DATA SET MUST BE PROVIDED TO CONTINUE EXECUTION. IF THE LOG DATA SET IS NOT SPECIFIED, NO LOG WILL BE WRITTEN. IF THE INPUT DATA SETS ARE NOT SPECIFIED, THE CARD READER WILL APPEAR NOT READY TO THE CENTRAL SITE.

THE PRINT DATA SET AND THE CARD READER DATA SET MAY BE SPECIFIED WITH SWITCHES. A LIST OF THIS SWITCHES MAY BE OBTAINED BY TYPING CONTROL-D FOLLOWED BY A COMMAND STRING INCLUDING THE SWITCH /HE ON THE PRINT DATA SET. AS MANY AS TEN SWITCHES MAY APPEAR ON ONE PRINT DATA SET, BUT ONLY

ONE SWITCH MAY APPEAR ON A CARD READER DATA SET.

THE VALID SWITCHES FOR THE PRINT DATA SET ARE:

/KB - ECHO KEYBOARD TO PRINTER

WHEN THIS SWITCH IS GIVEN WITH A PRINT DATA SET, THEN ALL LINES DIRECTED BY THE CENTRAL SITE TO THE CONSOLE ARE ALSO COPIED TO THE PRINT DATA SET. THIS SWITCH IS TURNED OFF WHENEVER A NEW PRINT DATA SET IS SPECIFIED.

/KB:N - DON'T ECHO KEYBOARD TO PRINTER

/BU: - CLEAR PRINT BURST LOGIC

THIS SWITCH CLEARS THE SPECIAL PRINT BURST LOGIC SET BY THE NEXT TWO SWITCHES. THE SYSTEM IS INITIALLY IN THIS STATE.

/BU:E - BURST ON END-OF-FILE

WHEN THIS SWITCH IS SET, IF THE CENTRAL SITE TRANSMITS AN END-OF-FILE TO THE TERMINAL PRINTER, THE CURRENT PRINT DATA SET WILL BE CLOSED, AND A NEW ONE REQUESTED. THIS SWITCH HOLDS UNTIL EXPLICITLY OVERRIDDEN.

/BU:N - BURST ON NAME

WHEN THIS SWITCH IS SET, THE CURRENT PRINT DATA SET WILL BE CLOSED WHENEVER THE CENTRAL SITE TRANSMITS AN END-OF-FILE, OR A LINE WITH THE CURRENT END-OF-RECORD CHARACTER (DEFAULT #) IN THE FIRST PRINTABLE POSITION. THE REMAINDER OF THE LINE IS TAKEN AS A NEW PRINT DATA SET SPECIFICATION

/CO - SET ASCII CODE

/CO:E - SET EXTERNAL BCD CODE

/CO:I - SET INTERNAL BCD CODE

/DE - SET DEBUG MODE

WHEN THIS SWITCH IS SET, TRANSMISSION ERRORS WILL CAUSE MESSAGES OF THE FORM ERRNNN TO BE PRINTED AT THE CONSOLE. IT HOLDS UNTIL DEFEATED. THE EXACT MEANING OF THE MESSAGES CAN BE FOUND IN THE SECTION ON UTILITY ROUTINES IN THE INTERNAL DOCUMENTATION.

/DE:N - TURN OFF DEBUG MODE

/CC - USE CARRIAGE CONTROL (DEFAULT)

/CC:N - DEFEAT CARRIAGE CONTROL

THIS SWITCH HAS EFFECT ONLY FOR THE CURRENT SPECIFICATION. THAT IS, IT MUST BE GIVEN EXPLICITLY EVERY TIME IT IS WANTED.

/CC:F - USE FOCUS CARRIAGE CONTROL

THIS SWITCH SETS UP CARRIAGE CONTROL FOR A NON-STANDARD BNL SYSTEM, FOCUS. IT SHOULD NOT BE USED IN GENERAL.

/SI - USE SITE ADDRESS FROM CENTRAL (DEFAULT)

/SI:NNN - USE SITE ADDRESS NNN

/ON - READ INPUT STRING ONLY ONCE

/ON:N - READ INPUT STRING REPEATEDLY (DEFAULT)

NORMALLY THE PROTOCOL WILL RESTART THE CARD READER DATA SET SPECIFICATIONS AFTER RUNNING TO THE END. WHEN THE /ON SWITCH IS USED A NEW COMMAND STRING MUST BE ENTERED BEFORE THE CARD READER DATA SET SCAN WILL BE RESTARTED. /ON:N UNDOES THIS RESTRICTION.

/RE - FORCE READ OF INPUT DATASET

THIS SWITCH FORCES THE FIRST READ OF THE CARD READER DATA SET BEFORE ANY REQUEST FROM CENTRAL. THIS IS EQUIVALENT TO THE F1 SWITCH ON A CDC 734.

/RW:N - DEFEAT MAGTAPE REWINDS

/RW:Y - ALLOW MAGTAPE REWINDS (DEFAULT)

/LM - SET LINE MODE (DEFAULT)

/BM - SET BLOCK MODE

/HE - PRINT INSTRUCTIONS

/ER - USE # AS END-OF-RECORD CHARACTER

/ER:NNN - USE CODE NNN AS END-OF-RECORD CHARACTER

THIS SWITCH SETS THE CODE TO BE USED ON CARD READER END-OF-RECORD CARDS, AND IN THE /BU:N LOGIC. FOR EXAMPLE, /ER:45 WOULD ALLOW A % TO FUNCTION AS THE END-OF-RECORD CHARACTER, WHILE /ER:0 WOULD PREVENT ALL USE OF END-OF-RECORD CARDS.

/EN - END CURRENT CARD READ FILE

THIS SWITCH CAUSES THE CURRENT CARD READ FILE TO BE PREMATURELY TERMINATED. NOTE THAT THIS SWITCH MUST APPEAR ON THE OUTPUT DATA SET, NOT THE CARD READER DATA SET SPECIFICATION.

/FO - SET FOCUS MODE (OBOLETE)

/FO:N - DEFEAT FOCUS MODE (DEFAULT)

TWO SWITCHES ARE ALLOWED FOR CARD READER DATA SETS: /NR AND /EF. THE FIRST CAUSES TRANSMISSION OF THE NEXT CARD READER DATA SET TO START WITHOUT THE TRANSMISSION OF AN END-OF-RECORD CARD, WHILE THE SECOND FORCES TRANSMISSION OF AN END-OF-FILE CARD. ONLY ONE OF THESE TWO SWITCHES MAY APPEAR ON A GIVEN CARD READER DATA SET.

YOU MAY MAKE THE PROGRAM REVERT TO COMMAND MODE AND WAIT FOR FOR A COMMAND STRING. A SECOND CONTROL-D WILL TERMINATE THE PROGRAM. COMMAND STRINGS MAY ALSO BE INPUT ON THE FLY BY STARTING THE LINE WITH CONTROL-A.

IF YOU WISH TO CHANGE ONLY SWITCH SETTINGS AND THE CARD READER DATA SET SPECIFICATIONS, USE THE PRINT DATA SET NC:, WHICH WILL LEAVE THE CURRENT PRINT DATA SET UNCHANGED.

AMD - CDC 200 UT SIMULATOR
CRYSNET UTILITY PROGRAM INSTALLATION INSTRUCTIONS

TO INSTALL THIS PACKAGE FROM THE RELEASE MEDIUM, ONE SHOULD BE RUNNING UNDER DOS, BE LOGGED IN UNDER UIC 1,1, AND HAVE THE DEC DOS/BATCH RELEASE MATERIALS AVAILABLE. WE WILL DESCRIBE A FULL INSTALLATION FROM SCRATCH. OF COURSE ONE MAY SKIP THE CREATION OF FILES FOR WHICH THE ONES ON THE RELEASE MEDIUM SATISFY LOCAL REQUIREMENTS. IN PARTICULAR, THE ASSEMBLY STEPS FOR AMD, MATCHR, AND KB, MAY BE SKIPPED FOR ALMOST ALL INSTALLATIONS, AND THE ASSEMBLY STEP FOR MR MAY BE SKIPPED IF THE DP11/DU11 TO BE DRIVEN IS THE FIRST AND HAS INTERRUPT VECTORS AT 300.

IN ALL THAT FOLLOWS, WE WILL USE "MR." IN PLACE OF EITHER "DP." OR "DU." HOWEVER, BE WARNED THAT MR WITHOUT A FOLLOWING PERIOD REALLY MEANS JUST THAT. THE SYSTEM KNOWS EITHER DRIVER AS DV.MR.

WE ASSUME YOU HAVE ONE MAGTAPE DRIVE, AND A COPY OF THIS RELEASE AND THE DEC RELEASE ON MAGTAPE. IF NOT, SUBSTITUTE THE APPROPRIATE DEVICE FOR MT0: IN ALL THAT FOLLOWS.

1. BRING FILES ONTO THE DISK FOR ASSEMBLIES AND EDITS.

```
$RUN PIP
... MOUNT THE AMD RELEASE TAPE ...
#SY:<MT0:MATCHR.MAC,AMD.MAC,MR.MAC,KB.MAC
... NOW DISMOUNT THE AMD RELEASE TAPE AND MOUNT DEC RELEASE
TAPE ...
#SY:<MT0:RMON.LDA,RMON.STB,TAILB.LDA,SYSTEM.MAC,CONFIG.MAC,CFM
C.MAC
#SY:<MT0:PRAMTR.MAC,FEATSW.MAC
#↑C
.KI
```

2. PERFORM EDITS OF SYSTEM.MAC, MR.MAC.

```
$RU EDIT
#SYSTEM.MAC<SYSTEM.MAC
*R
*G,UDDEV=,1C,1,
...NOTE THAT WE JUST SAID 1 USER DEFINED DEVICE...
*G,.MACRO,G,<,I/<MR,300,174770>/
...NOTE THAT 300 IS THE INTERRUPT VECTOR FOR THE DP11
...AND 174770 IS THE MODEM RECEIVE STATUS,
...(160010 SHOULD BE USED FOR DU11)
...WHICH WOULD NOT BE GIVEN IN AN 08-08 SYSTEM
...BE SURE THESE NUMBERS MATCH YOUR HARDWARE...
*EX
...NOTE THAT UNDER 08-08 THE DEFINITION OF GDVU2 IS MISSING
...YOU REALLY SHOULD PUT IT IN BEFORE THE EX...
#MR.MAC<MR.MAC
*R
...NOTE THAT THE NEXT LINES ARE JUST FOR DP.MAC ...
*G,174770,-6C,174770,
*G,174772,-6C,174772,
*G,174774,-6C,174774,
```

```
*G,174776,-6C,174776,
*G,300,-3C,300,
*G,304,-3C,304,
...SUBSTITUTE YOUR DP11 REGIISTERS AND VECTORS IN
...THE RIGHT HALF OF EACH COMMAND...
*EX
...THIS IS THE END OF THE DP11 PATCHES ...
... THE FOLLOWING IS JUST FOR DU.MAC ...
*R
*G,DUREGS,
*G,160010,-6C,160010,
*G,304,-3C,304,
...SUBSTITUTE YOUR DU11 REGISTERS AND XMIT VECTOR ...
*EX
...THIS IS THE END OF THE DU11 PATCHES...
↑C
.KI
```

3. ASSEMBLE ALL MODULES.

```
$RUN MACRO
#CFTBL.OBJ/EN:CDR<CFMAC,SYSTEM,CONFIG
...YOU'LL BOMB HERE IF YOU DON'T HAVE FIXES OF DIGITAL
...SOFTWARE NEWS, DEC 73, DOS-11 #37 INSTALLED IN 08-08...
#AMD/EN:CDR<AMD
#MATCHR/EN:CDR<MATCHR
#KB/EN:CDR<PRAMTR,FEATSW,KB
#MR/EN:CDR<MR.MAC
#↑C
.KI
```

4. PERFORM ALL LINKS.

```
$RUN LINK
#CFTBL<RMON.STB,CFTBL/B:0/E
#AMD<AMD/B:34000/E
#KB<KB,MATCHR/B:0/E
#MR<MR/B:0/E
#↑C
.KI
```

5. CLEAN UP WITH PIP A BIT.

```
$RU PIP
#*.BAK/DE
#MATCHR.MAC/DE
#AMD.MAC/DE
#MR.MAC/DE
#KB.MAC/DE
#FEATSW.MAC/DE
#PRAMTR.MAC/DE
#SYSTEM.MAC/DE
#CFMAC.MAC/DE
#CONFIG.MAC/DE
#RMON.STB/DE
#CFTBL.OBJ/DE
#MATCHR.OBJ/DE
#AMD.OBJ/DE
```

```
#MR.OBJ/DE
#KB.OBJ/DE
#USER.LDA<KB.LDA,MR.LDA
#KB.LDA/DE
#MR.LDA/DE
#↑C
.KI
```

6. BUILD A NEW MONITOR CIL.

```
$RUN CILUS
#,,NEWMON.LCL<RMON/BU,CFTBL,TAILB/E
#NEWMON.CIL<NEWMON.LCL,USER/E
*R DV.KB:DV.KB
*I DV.MR
*E
#NEWMON.CIL/BO
...NOW YOU SHOULD BE ABLE TO LOG IN AND RUN AMD
...IF ALL IS WELL COME BACK TO CILUS AND HOOK NEWMON.CIL...
#NEWMON.CIL/HO
```

7. CLEAN UP EXTRA FILES.

```
$RUN PIP
#USER.LDA/DE
#CFTBL.LDA/DE
#RMON.LDA/DE
#TAILB.LDA/DE
#NEWMON.BAK/DE
```

NOW YOU ARE DONE, WE HOPE.

AMD - CDC 200 UT SIMULATOR
INTERNAL DOCUMENTATION FOR AMD.MAC

THE ORIGINAL VERSION OF THIS INTERNAL DOCUMENTATION WAS PREPARED BY G. H. CAMPBELL OF THE APPLIED MATHEMATICS DEPARTMENT.

THIS IS THE INTERNAL DOCUMENTATION FOR THE PROGRAM AMD, A SIMULATOR FOR A CDC 200 USER TERMINAL. PLEASE NOTE THAT THERE IS NO IMPLEMENTATION OF THE MESSAGE TYPE DIAGNOSTIC WRITE, AND THAT A BUFFER LOAD OF CARDS CAN CONSIST OF FEWER THAN 12 CARD IMAGES.

1. NOTATION CONVENTIONS USED.

THE FIRST TWO CHARACTERS OF A NAME OF THE BUFFER AREAS, ETC. ARE HD FOR LINE BUFFER HEADER, AB FOR THE ACTUAL BYTE-COUNT ENTRY IN THE LINE BUFFER HEADER, BF FOR THE BEGINNING OF LINE BUFFER, LK FOR THE LINK BLOCK, FI FOR THE FILE BLOCK. THE LAST TWO CHARACTERS ARE LP FOR THE DATA STREAM OUTPUT, CR FOR THE DATA STREAM INPUT, KI FOR THE CONSOLE INPUT, AND KO FOR THE CONSOLE OUTPUT; MR FOR THE MODEM INPUT, MS FOR THE MODEM OUTPUT. CIRCULAR BUFFERS ARE DEFINED BY A TWO-CHARACTER DEVICE MNEMONIC, THE LETTER Z AND ANOTHER TWO CHARACTER DEVICE MNEMONIC INDICATING THE DIRECTION OF DATA FLOW THROUGH THAT CIRCULAR BUFFER. THE CIRCULAR BUFFER POINTERS ARE DEFINED BY THE BUFFER NAME FOLLOWED BY AN F, I, O, OR L FOR FIRST, IN, OUT, OR LIMIT.

FOUR MACROS ARE USED TO IMPROVE READABILITY: CALL, RETURN, PUSH, AND PULL. THEY ARE DEFINED ON LINES AMD$.72 THROUGH AMD$.95. A PC CALLING SEQUENCE IS USED WITHOUT AN ARGUMENT LIST.

THE MAJOR CONSTANTS USED BY THE PROGRAM ARE DEFINED BETWEEN LINES AMD$.96 AND AMD$.164. EXCEPT FOR THE FOLLOWING, IT IS NOT RECOMMENDED THAT THEY BE CHANGED. THE SYMBOL EORA (AMD$.135) DEFINES THE DEFAULT FOR THE CHARACTER TO FLAG AN END-OF-RECORD CARD. IT MAY BE CHANGED TO ANY SUITABLE CHARACTER. IN PARTICULAR, IF ONE USES 029 PUNCH CARDS, CHANGING TO 76 (!>) WOULD MAKE THE 7-8-9 CARD AN END-OF-RECORD CARD IN THIS MODE. MOST OF THE BUFFER LENGTHS MAY BE CHANGED, BUT WITH CAUTION. THE MODEM BUFFERS MAY BE SHORTENED FOR CENTRAL SITES THAT WILL TOLERATE THIS, BY REDUCING LBMD (AMD$.148) AND LWMD (AMD$.149) KEEPING A TWO TO ONE RATIO, AND CUTTING NCPT (AMD$.163) TO THE MAXIMUM NUMBER OF CARD IMAGES. THE PROGRAM MAY BE MADE CONSIDERABLY SMALLER BY REDUCING THE SIZE OF THE CIRCULAR BUFFERS CONTROLLED BY LBMK (AMD$.156) AND LBLC (AMD$.157). BE CERTAIN TO LEAVE ENOUGH ROOM FOR TWO CARD IMAGES (162. CHARACTERS).

THE MAJOR FLAGS AND VARIABLES USED BY THE PROGRAM ARE DEFINED BETWEEN LINES AMD$.166 AND AMD$.205. THOSE BETWEEN SGLB AND EGLB ARE CLEARED ON PROGRAM START OR RESTART. IT SHOULD BE NOTED THAT THE LOCATION SWID (AMD$.204) DEFINES THE SCREEN WIDTH IN TERMS OF LBKO. IF ONE HAS A CONSOLE WHICH CAN PRINT FEWER THAN 80 CHARACTERS ON A LINE, SWID SHOULD BE RESET, EITHER BY REDEFINING LBKO, OR BY CHANGING THIS LINE.

2. OVERVIEW OF DATA FLOW

THE PROGRAM MUST MANAGE DATA FOLOWS IN THE FOLLOWING DIRECTIONS: FROM THE CENTRAL SITE TO THE TERMINAL CONSOLE, FROM THE CENTRAL SITE TO THE

TERMINAL LINE PRINTER, FROM THE TERMINAL CONSOLE TO THE CENTRAL SITE, FROM THE TERMINAL CARD READER TO THE CENTRAL SITE, FROM THE TERMINAL CONSOLE TO THE PROGRAM ITSELF (TO CONTROL OPERATION OF THE PROGRAM), AND FROM THE PROGRAM TO THE TERMINAL CONSOLE (TO INFORM THE OPERATOR OF INTERNAL STATES).

THE CIRCULAR BUFFERS PROVIDE THE MAIN HOLDING AREAS FOR DATA. EACH CIRCULAR BUFFER HAS A SET OF POINTERS ASSOCIATED WITH IT TO CONTROL ITS USE: FIRST, IN, OUT, AND LIMIT. THE BUFFER CONSISTS OF THE MEMORY FROM FIRST THROUGH LIMIT-1. DATA IS ENTERED AT IN, AND REMOVED AT OUT. THE BUFFER IS EMPTY WHEN IN=OUT, AND FULL WHEN IN=OUT-1. DATA FLOWS FROM DEVICE ORIENTED BUFFERS INTO AND OUT OF THE CIRCULAR BUFFERS. FOR EXAMPLE, CONSIDER THE CASE OF DATA OUTPUT. DATA COMES IN TO A BUFFER ASSOCIATED WITH A MODEM, IS MOVED TO A CIRCULAR BUFFER, MDZLP, INDICATING IT IS IN TRANSIT FROM THE MODEM TO THE LINE PRINTER, AND THEN IS UNPACKED LINE-BY-LINE FROM THAT BUFFER INTO A LINE BUFFER FOR THE LINE PRINTER. THIS SAME PHILOSOPHY IS APPLIED TO THE OTHER THREE DATA STREAMS. DATA IN THE CIRCULAR BUFFERS IS HELD IN THE FORMAT THAT THE MODEM DRIVERS EXPECT TO FIND IT. ANY REFORMATTING THAT IS NECESSARY IS DONE BETWEEN THE DOS LINE BUFFER AND THE CIRCULAR BUFFER.

THE CONTROL FLOW IS GOVERNED BY A SMALL MAIN PROGRAM WHICH SIMPLY CALLS IN SUCCESSION SUBROUTINES FOR HANDLING THE MODEM, CARD READER, LINE PRINTER, KEYBOARD RECEIVE, AND TELETYPE PRINT. EACH OF THESE SUBROUTINES TESTS A DEVICE FOR BEING READY, AND IF IT IS READY, INITIATES THE NEXT TRANSACTION WITH THAT DEVICE, IF THERE IS ONE. IN GENERAL, THESE ARE STRUCTURED AS A SMALL CONTROL ROUTINE TO TEST FOR AN ACTIVITY THAT SHOULD NOW BE INITIATED ON THAT DEVICE, AND UPON DISCOVERING SOME ACTIVITY, THEN CALLS ANOTHER PROGRAM WHICH IN FACT DOES IT. A PECULIARITY OF THIS CODE TO BE MENTIONED NOW, IS THE MANNER OF HANDLING KEYBOARD INPUT- OUTPUT. SINCE STANDARD DOS ALLOWS ONLY ONE OPERATION IN ONE DIRECTION AT ONE TIME, WE MUST USE THE REVISED KB DRIVER TO REMOVE THAT RESTRICTION.

3. THE KEYBOARD RECEIVE PROCESSOR.

THE PORCESSOR HANDLES THE DATA FLOW FROM THE TERMINAL CONSOLE KEYBOARD TO EITHER THE CENTRAL SITE, OR THE PROGRAM ITSELF. IF A LINE IS INTENDED FOR THE CENTRAL SITE, IT IS PASSED ON TO THE ROUTINE MLK (AMD$.578 THROUGH AMD$.604). IF THE LINE IS INTENDED FOR THE PROGRAM ITSELF, IT IS PROCESSED BY CSI (AMD$.606 THROUGH AMD$02.40). LINES INTENDED FOR THE PROGRAM MAY BE ENTERED BY FIRST TRAANSMITTING AN END-OF-MEDIUM FROM THE KEYBOARD (CONTROL-D OR CONTROL-C, END) AND THEN TYPING THE LINE FOR THE PROGRAM, OR BY SIMPLY STARTING THE LINE WITH CONTROL-A. KRP RECOGNIZES THE END-OF-MEDIUM STATUS, RELEASES THE DRIVER, AND INITIALIZES A NEW ONE WITH THE NAME CMI. IT THEN READS ONE LINE FOR CSI, AND REVERTS BACK TO THE NAME PCI. IF THAT LINE READ CAUSES A SECOND END-OF-MEDIUM, KRP TERMINATES THE PROGRAM IMMEDIATELY. IF THE LINE IS NOT SO FLAGGED FOR THE PROGRAM AND IF THERE IS ROOM IN THE CIRCULAR BUFFER, IT IS MOVED TO THE CIRCULAR BUFFER, AND ANOTHER READ INITIATED. IN THE PROCESS OF MOVING DATA TO THE CIRCULAR BUFFER ALL CONTROL CHARACTERS, OTHER THAT TAB ARE IGNORED. A LINE IS TERMINATED BY A CARRIAGE RETURN, LINE FEED, OR FORM FEED. TABS ARE CONVERTED TO 1-8 BLANKS TO MOVE TO COLUMNS 9, 17, 25, ETC.

THE CSI MODULE MAY BE ENTERED AT CSI TO MOVE A LINE FROM THE KEYBOARD BUFFER TO THE COMMAND BUFFER (STRIPPING THE FIRST CHARACTER), OR AT CSI4 TO PROCESS A LINE ALREADY THERE. THE SWITCHES FOR THE FIRST OUTPUT DATA SET ARE MATCHED AGAINST THE LIST AT CSISW (AMD$.611). ANY THAT MATCH ARE INTERPRETED BY THE EXECUTION ROUTINES IN THE SAME LIST. NO ERROR IS REPORTED FOR FAILURE TO MATCH. IF A NEW PRINT DATA SET IS GIVEN THE OLD ONE IS CLOSED, BUT THE NEW ONE IS NOT YET OPENNED. NO ACTION IS TAKEN ON THE CARD READER DATA SETS, UNLESS THE SWITCH /EN IS USED ON THE PRINT DATA SET. ANY EXISTING LOG DATA SET IS CLOSED, AND THE NEW ONE, IF GIVEN, IS OPENNED.

THE PRINT DATA SET SWITCHES ARE HANDLED BY THE ROUTINES ECKB, SCOD, SDEB, SSITE, SLM, SBM, CARCON, SEOR, HELP, ENDCR, SFO AND SBU (AMD$.746 THROUGH AMD$02.40). THE COMMENTS IN THE LISTING SHOULD BE CONSULTED FOR DETAILS. EACH IS A SUBROUTINE WHICH ASSUMES THAT R0 POINTS TO THE FIRST VALUE, WHILE R1 HAS A COUNT OF THE VALUES.

4. THE TELETYPE PRINT PROCESSOR.

THIS PROCESSOR HAS TO CHECK FOR MESSAGES TO BE TYPED FROM A VARIETY OF DIFFERENT SOURCES. IF THE DEBUG SWITCH IS SET, YOU MUST CHECK FOR ERROR TYPE-OUTS, OR FREE MEMORY TYPE-OUTS, AS WELL AS THE NORMAL KEYBOARD OUTPUT STREAM. THE ERROR TYPE-OUTS COME FROM THREE POTENTIAL SOURCES. ONE IS THE MODEM DRIVER ERROR REPORTING BUFFER. ANOTHER IS THE FREE MEMORY REPORTING BUFFER, AND A THIRD IS THE GENERALIZED ERROR MESSAGE REPORTING BUFFER. ALL OF THESE WILL BE COVERED SEPARATELY. IN MOVING CONSOLE OUTPUT TO THE TELETYPE BUFFER, A CARRIAGE RETURN LINE FEED IS INSERTED UPON DETECTING EITHER AN EOL OR A CARRIAGE RETURN CODE AND THE LINE IS COMPLETED FOR OUTPUT. UPON DETECTION OF AN END OF FILE, A FORM FEED IS EMITTED. THE LOCATION CSTRT IS USED TO HOLD THE CURRENT LINE POSITION. WHEN THE NUMBER OF CHARACTERS ON A LINE IS AT LEAST THE VALUE HELD IN SWID, THE LINE IS TERMINATED AND PRINTED, AND A NEW LINE STARTED. IN ALL CASES, TRAILING BLANKS ARE STRIPPED.

5. THE LINE PRINTER PROCESSOR.

IN ORDER TO HANDLE THE CARRIAGE CONTROL CORRECTLY AN UNUSUAL PHILOSOPHY IS ADOPTED IN FORMATTING LINES FOR PRINTING. EACH LINE BEGINS WITH THE LINE TERMINATORS NECESSARY FOR THE PREVIOUS LINE, PLUS ANY NECESSARY CARRIAGE CONTROL FOR THE CURRENT LINE. COMPRESSED ZEROS AND BLANKS ARE EXPANDED DURING FORMATTING OF THE PRINT LINE IMAGE. IN DETAIL, THE ACTION TAKEN ON ENCOUNTERING THE CARRIAGE CONTROL CHARACTER IS AS FOLLOWS: A CARRIAGE RETURN IS INSERTED IN THE BUFFER; THEN FOR SINGLE SPACE, A LINE FEED IS INSERTED; FOR DOUBLE SPACE, TWO LINE FEEDS ARE INSERTED. FOR PAGE EJECT A FORM FEED IS INSERTED, AND FOR SUPPRESS SPACE A VERTICAL TAB IS INSERTED (UNLESS THIS IS THE VERY FIRST LINE OF THE FILE, IN WHICH CASE NOT LEADING CARRIAGE CONTROL IS USED FOR SUPPRESS SPACE). IF THE FIRST CHARACTER OF THE LINE IS AN ESCAPE, IT MIGHT GENERATE ZEROS OR BLANKS, SO THE LINE IS CONSIDERED NOT YET TO HAVE A FIRST CHARACTER.

THE CARRIAGE CONTROL SET USED IS DETERMINED BY THE CODE SET, AND IS PICKED UP FROM LOCATIONS CARC, CARC+1, AND CARC+2 FOR DOUBLE SPACE, EJECT, AND SUPPRESS SPACE RESPECTIVELY. THE VALUES THE TERMINAL SEES

ARE:

ASCII	BCD	FUNCTION
J	0	DOUBLE SPACE
A	1	PAGE EJECT
0	+	SUPPRESS SPACE

ALL OTHER CHARACTERS ARE TREATED AS SINGLE SPACE CONTROL.

6. THE CARD INPUT PROCESSOR.

IN ORDER TO AVOID DOS TAKING CONTROL AWAY ON DEVICE NOT READY CONDITIONS, THAT CARD INPUT PROCESSOR IS COMPLETELY SHORT- CIRCUITED UNLESS A FLAG RMC (FOR READ MORE CARDS) IS SET. THIS FLAG IS SET ONLY BY A CENTRAL SITE REQUEST FOR CARD INPUT DATA. IF THIS FLAG IS SET AND IF THERE IS ROOM IN THE CIRCULAR BUFFER FOR ANOTHER CARD IMAGE, THEN A TEST IS MADE TO SEE IF WE HAVE AN INPUT DATA SET DEFINED. IF THERE IS NO INPUT DATA SET CURRENTLY ACTIVE, WE SET A FLAG TO ASSUME THE CARD READER IS NOT READY, AND CALL THE ROUTINE NEXTIN TO ANALYSE THE STORED COMMAND STRING. THE ROUTINE NEXTIN, SIMPLY CALLS CSI2, ASKED IT TO SET UP THE LINK BLOCK AND FILE BLOCK FOR THE NEXT INPUT FILE. IT RETURNS A FLAG INDICATING EITHER NO VALID COMMAND STRING AVAILABLE OR THERE IS NO NEXT ENTRY, OR THE NEXT ENTRY IS CURRENTLY SET UP. IF THERE IS NO VALID COMMAND STRING, THEN AN IMMEDIATE EXIT IS TAKEN FROM THE ROUTINE, LEAVING THE CARD READER NOT READY FLAG SET. IF THERE IS NO NEXT ENTRY THEN CSI1 IS CALLED TO RESTART THE ANAYLSIS OF THIS COMMANDSTRING FROM THE BEGINNING AND NEXTIN IS CALLED AGAIN. IF AT THIS POINT THERE IS STILL NO VALID COMMAND STRING OR NO VALID NEXT ENTRY, AN EXIT IS TAKEN, LEAVING THE CARD READER NOT READY FLAG SET. OTHERWISE, THE CARD READER NOT READY FLAG IS CLEARED AND THE NEXT DATA SET IS INIT'ED, OPENED, A READ INITIATED, AND A RETURN TAKEN. IF UPON ENTRY, THERE WAS AN ACTIVE DATA SET AND THE READ FOR THAT DATA SET HAS BEEN COMPLETED, IT IS TESTED FOR BEING AN END-OF-FILE. ON AN END-OF-FILE CONDITION THAT DATA SET IS CLOSED AND RELEASED, AND THE NR SWITCH IS TESTED TO DETERMINE WHETHER TO SEND AN END-OF- RECORD AT THIS POINT OR NOT. IN EITHER CASE, NEXTIN IS AGAIN CALLED, AND IF ANOTHER DATA SET IS AVAILABLE IN THE COMMAND STRING IT IS INIT'ED OPENED AND A READ IS ISSUED. IF THERE ARE NO MORE DATA SETS AVAILABLE, AN END-OF-FILE IS PUT INTO THE BUFFER, AND THE READ-MORE-CARDS FLAG IS CLEARED. IF WE ARE NOT AT END-OF-FILE THEN THE FIRST CHARACTER ON THE NEXT CARD IS CHECKED. IF THIS CHARACTER IS A 43-OCTAL, THEN THIS IS ASSUMED TO BE AN END-OF-RECORD FLAG AND AN END-OF-RECORD CARD IMAGE IS OUTPUTTED. OTHERWISE, THE CARD IMAGE IS SIMPLY MOVED TO THE CIRCULAR BUFFER, IGNORING ANY CONTROL CHARACTERS, AND BLANK PADDING TO 80 COLUMNS.

7. THE MODEM PROCESSOR.

THE MODEM PROCESSOR WORKS IN CONJUNCTION WITH THE PROCESS INPUT MESSAGE ROUTINE TO HANDLE THE MODEM DIALOGUE. IF AN OUTPUT IS IN PROGRESS, IT TESTS TO SEE IF IT IS COMPLETE, AND IF SO, INITIATES AN INPUT. IF AN INPUT IS IN PROGRESS, IT TESTS TO SEE IF IT IS COMPLETE, AND IF IT IS COMPLETE, CALLS THE PIM ROUTINE WHICH WILL PROCESS THE

INPUT MESSAGE AND INITIATE THE NEXT OUTPUT. THE PROCESS INPUT MESSAGE ROUTINE FIRST CALLS ANOTHER ROUTINE TO CHECK THE FORMAT OF THE MESSAGE AS WELL AS SET CERTAIN FLAGS FOR THE TYPE OF MESSAGE READ AND THE TERMINATING E CODE. OUTPUT VARIABLES FROM THIS ROUTINE ARE THE SWITCH TMI, WHICH IS ZERO IF A POLL WAS RECEIVED, ONE IF A WRITE WAS RECEIVED; ESCW, WHICH IS -1 FOR AN E1, 0 FOR AN E2, AND +1 FOR AN E3 TERMINATOR. ADDITIONALLY, THE VARIABLE NBDI IS SET TO INDICATE THE NUMBER OF DATA BYTES IN THE MESSAGE. THHE FORMAT CHECK ROUTINE ALSO TESTS ANY ERROR STATUS RETURNED BY THE DRIVER. IF THE RESULT OF THE FORMAT CHECK IS AN ERROR, A NAK RESPONSE IS SENT. (N.B. THE FORMAT CHECK ROUTINE ALSO ESTABLISHES THE SITE CODE TO BE USED IN RESPONSES BY THE FIRST VALID MESSAGE IT RECEIVES. THUS THIS SIMULATOR CAN BE USED ON A MULTI-DROP LINE WITHOUT MODIFICATION, BUT ONLY IF NO OTHER TERMINAL WILL CONTEND.) THE ACTION OF THE PROCESS INPUT MESSAGE ROUTINE CAN BEST BE UNDERSTOOD BY REFERENCE TO THE CODE. THE FOLLOWING THING SHOULD BE NOTED. THE MAXIMUM NUMBER OF CARDS TO BE SENT IN A GIVEN BLOCK IS DEFINED BY THE ASSEMBLY TIME PARAMETER NCPT. AN E2 RESPONSE TO A READ-MORE-CARDS REQUEST IS GIVEN ONLY IF THERE IS NO DATA AVAILABLE IN THE BUFFER, AND THE CARD READER NOT-READY FLAG IS SET. ANOTHER CHARACTERISTIC IS THAT AT ANY POINT WHERE AN AUTO-READ CAN BE SET UP, A CONSOLE MESSAGE MAY BE SENT INSTEAD, IF ONE IS WAITING.

IN ORDER TO PREVENT LOOPS OF REREADS OF THE CARD READER DATA SET, THE FLAG CNR IS SET NEGATIVE WHEN THE LAST DATA SET SPECIFICATION HAS BEEN PROCESSED BY CIP. PIM TRANSMITS E2 READ MESSAGES IN THIS CASE TO INFORM THE CENTRAL SITE THAT THE CARD READER IS NOT READY, AND FORCES RMC CLEAR TO KEEP CIP FROM READING ANY MORE CARDS, DESPITE THE CENTRAL REQUEST. THE SITUATION CAN BE CLEARED ONLY BY KRP, WHICH CHANGES CNR FROM NEGATIVE TO POSITIVE WHEN A NON-COMMAND INPUT LINE IS READ.

THE CONVERSIONS FOR THE CHARACTER SET CHOSEN ARE DONE BY THE ROUTINES WRMOD (AMD$.1385 - AMD$.1452) AND TMREAD (AMD$.1536 - AMD$.1579) USING THE TABLES SET UP BY THE MACRO CHTAB AND ITS CALLS (AMD$.1453-AMD$.1535). NO BIAS IS USED, SO THE TABLES ALLOW FOR FULL 128 CHARACTER CONVERSIONS, EVEN THOUGH ONLY 64 CHARACTERS ARE USED. WRMOD CONVERTS MESSAGES FROM THE TERMINAL TO CENTRAL FROM ASCII TO BCD IF NECESSARY, TRANSMITTING THE ASCII FROM BFMS, OR THE BCD FROM BFMS2. TMREAD TRANSLATES IN PLACE IN BFMRD FROM BCD TO ASCII, IF NECESSARY, USING THE ESCAPE CHARACTER TO FLAG THE MESSAGE CODE (33 FOR ASCII, 76 FOR EXTERNAL BCD, 136 FOR INTERNAL BCD). ONLY 63 CHARACTERS ARE VALID IN THE BCD SET. FUNCTION SEQUENCES ARE FLAGGED BY AN ESCAPE. IF THE CODE IS EXTERNAL BCD, THE FUNCTION IS THE SAME AS IN THE ASCII SET, EXCEPT THAT 120 IS CONVERTED TO 100. IF THE CODE IS INTERNAL BCD, THE FUNCTION IS CONVERTED FROM INTERNAL BCD TO EXTERNAL BCD, AND THEN TREATED AS EXTERNAL BCD. THE CHARACTER SETS USED ARE AS FOLLOWS:

ASCII	EXT	INT	ASCII	EXT	INT	ASCII	EXT	INT	ASCII	EXT	INT
SP 40	120	060	0 060	112	100	@ 100	115	115	P 120	047	047
! 041	052	052	1 061	101	101	A 101	061	121	Q 121	050	050
" 042	114	114	2 062	102	102	B 102	062	122	R 122	051	051
# 043	136	076	3 063	103	103	C 103	063	123	S 123	122	062
$ 044	053	053	4 064	104	104	D 104	064	124	T 124	123	063
% 045	116	116	5 065	105	105	E 105	065	125	U 125	124	064
& 046	137	077	6 066	106	106	F 106	066	126	V 126	125	065
' 047	055	055	7 067	107	107	G 107	067	127	W 127	126	066
(050	134	074	8 070	110	110	H 110	070	130	X 130	127	067
) 051	074	134	9 071	111	111	I 111	071	131	Y 131	130	070
* 052	054	054	: 072	100	112	J 112	041	041	Z 132	131	071
+ 053	060	120	; 073	077	137	K 113	042	042	[133	117	117
, 054	133	073	< 074	072	132	L 114	043	043	\ 134	075	135
- 055	040	040	= 075	113	113	M 115	044	044	] 135	132	072
. 056	073	133	> 076	057	057	N 116	045	045	↑ 136	---	---
/ 057	121	061	? 077	056	056	O 117	046	046	← 137	135	075

8. UTILITY ROUTINES.

THERE IS A SMALL ROUTINE WHICH, IF DEBUG MODE IS SET, COMPUTES THE FREE CORE AVAILABLE, AND SETS UP A TYPEWRITER OUTPUT OF THIS INFORMATION. THIS ROUTINE IS CALLED WHENEVER A NEW DATA SET IS INITIALIZED. THERE IS ALSO A SMALL ERROR PROCESSOR WHICH IS ENTERED WHENEVER AN ERROR IS DETECTED WITH AN APPROPRIATE ERROR CODE. IF THE DEBUG MODE IS SET, THIS ROUTINE STORES THAT ERROR CODE IN A TABLE FOR LATER OUTPUTTING BY TELETYPE PRINT PROCESSOR. IT HAS THE CHARACTERISTIC THAT IF THIS ERROR TABLE FILLS UP, IT CONTINUOUSLY STORES THE NEGATIVE OF THE LAST ERROR CODE, IN THE LAST LOCATION OF THIS TABLE, UNTIL IT BECOMES FREE AGAIN. POSSIBLE ERROR MESSAGES FOLLOW:

1. DRIVER REPORTED ERROR.

2. INPUT MESSAGE SMALLER THAN MINIMUM SIZE.

3. MESSAGE DOES NOT START WITH SOH.

4. ERROR IN SITE ADDRESS.

5. ERROR IN STATION ADDRESS.

6. UNRECOGNIZATBLE MESSAGE-TYPE CODE.

7. INPUT DOES NOT END WITH ETX.

8. NO ESCAPE E1, E2, OR E3 AT END OF WRITE MESSAGE.

20. SYNTAX ERROR IN COMMAND STRING.

21. TELETYPE LINE TOO LONG.

22. IMPROPER TERMINATION OF KEYBOARD LINE INPUT.

23. PRINT LINE TOO LONG. A PECULIARITY OF THE TYPE-OUT OF THE ERRORS REPORTED IN THIS TABLE IS THAT THE NEGATIVE VALES WHICH ARE STORED WHEN THE TABLE FILLS UP ARE CONVERTED IN OUTPUT AS DECIMAL FULL-WORD POSITIVE INTEGERS.

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BUFFER$

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

DEC PDP 11
DEC DOS/BATCH V8, V9

.GLOBL BUFFEI,BUFFEO

PURPOSE

BUFFER$ IS INTENDED TO PROVIDE ASYNCHRONOUS I/O CAPABILITIES FOR FORTRAN PROGRAMS.

INTRODUCTION

BUFFER$ IS AN ASSEMBLY LANGUAGE (MACRO-11) ROUTINE WITH ENTRY POINTS BUFFEI AND BUFFEO, WHICH FILL THE ROLES OF THE BUFFERIN AND BUFFEROUT STATEMENTS FOUND IN MOST FORTRAN COMPILERS. TO ALLOW FOR THE VARIABLE NUMBER OF BYTES PER ELEMENT IN BYTE, INTEGER, REAL, AND DOUBLE PRECISION ARRAYS, AN OPTIONAL FORMAL PARAMETER HAS BEEN PROVIDED IN WHICH ONE CAN SPECIFY THE NUMBER OF BYTES PER ELEMENT. THE DEFAULT OF ONE BYTE PER ELEMENT WILL CAUSE INCOMPATABILITIES WITH OTHER SYSTEMS, UNLESS A VARIABLE IS USED TO CARRY THE INFORMATION.

THE DESCRIPTION OF THIS CODE IS INCOMPLETE WITHOUT REFERENCE TO THE WRITEUP OF IOCHEK$.

USE

BUFFER$ IS CALLED TO START A READ OR A WRITE. CONTROL IS RETURNED BEFORE THE OPERATION IS NECESSARILY COMPLETE. THE CALLS ARE OF THE FORM:

```
CALL BUFFEI(IUN,IMOD,IA(1),IA(N) [,NBYT] )
CALL BUFFEO(IUN,IMOD,IA(1),IA(N) [,NBYT] )
```

WHERE BUFFEI IS CALLED TO START A READ, AND BUFFEO IS CALLED TO START A WRITE. THE PARAMETERS HAVE THE FOLLOWING MEANING:

IUN - LOGICAL UNIT NUMBER, THE FORTRAN UNIT NUMBER ON WHICH THE OPERATION IS TO BE DONE.

IMOD - THE MODE OF THE TRANSFER, 0 FOR ASCII, 1 FOR FORMATTED BINARY, 2 FOR UNFORMATTED ASCII, 3 FOR UNFORMATTED BINARY. THE USER SHOULD BE CAREFUL TO MATCH THE MODE TO HIS APPLICATION. NOTE THAT IMOD OF 0, FORMATTED ASCII IMPLIES THE TRANSFER OF THE LINE TERMINATION CHARACTERS (CR, LF) AS WELL AS THE DATA, AND THAT IMOD OF 1, FORMATTED BINARY, DOES NOT MATCH THE FORTRAN UNFORMATTED BINARY WRITE FORMAT, WHICH CONSISTS OF MULTIPLE FORMATTED BINARY RECORDS FOR EACH FORTRAN LOGICAL RECORD.

IA - THE ARRAY OF DATA TO BE READ OR WRITTEN.

N - THE DIMENSION OF THE ARRAY IA. THUS IA(1) IS THE FIRST ARRAY ELEMENT TO TRANSFER, AND IA(N) IS THE LAST ELEMENT TO TRANSFER. THE TRANSFER WILL MOVE A CONTIGUOUS CORE IMAGE.

NBYT - THE NUMBER OF BYTES PER ARRAY ELEMENT. THIS PARAMETER IS OPTIONAL. IF IT IS NOT GIVEN, THE ARRAY IS ASSUMED TO BE A BYTE ARRAY. OTHERWISE, GIVE NBYT OF 1 FOR A BYTE ARRAY, 2 FOR AN INTEGER ARRAY, 4 FOR A REAL ARRAY, AND 8 FOR A DOUBLE PRECISION ARRAY. THE USER IS ADVISED TO USE A VARIABLE STORED IN A COMMON FOR THE PARAMETER TO EASE CONVERSION OF CODE TO MACHINES WITH DIFFERENT WORD SIZES.

NOTE

THIS CODE CAN INTERFACE WITH FILES HANDLED BY THE STANDARD FORTRAN I/O STATEMENTS, BUT NOT WHILE A BUFFER OPERATION IS IN PROGRESS. RANDOM FILES CAN BE READ AND WRITTEN BY USING AN IMOD OF 3, TO MATCH THE STANDARD FORTRAN CONVENTION OF UNFORMATTED BINARY, AND SETTING THE ASSOCIATED VARIABLE TO THE DESIRED RECORD NUMBER. A DEFINE FILE STATEMENT SHOULD BE EXECUTED BEFORE THE FIRST BUFFER CALL. THE RECORD LENGTH IS TAKEN FROM THE ARRAY LENGTH AND SHOULD AGREE WITH THE ARRAY LENGTH IN THE DEFINE FILE STATEMENT, OR THE FILE MAY BE GROSSLY MISPOSITIONED.

IOCHEK$

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

DEC PDP 11
DEC DOS/BATCH V8, V9

.GLOBL IOCHEK, LENGTH

PURPOSE

IOCHEK$ PROVIDES ROUTINES TO CHECK THE STATUS OF ASYNCHRONOUS INPUT-OUTPUT OPERATIONS FROM FORTRAN.

INTRODUCTION

IOCHEK$ IS AN ASSEMBLY LANGUAGE ROUTINE (MACRO-11) PROVIDING THE COMPANION ROUTINES TO BUFFER$, SO THAT ONE CAN CHECK FOR COMPLETION OF AN ASYNCHRONOUS I/O, AND DETERMINE THE AMOUNT OF DATA READ.

USE

TWO FUNCTIONS ARE PROVIDED, IOCHEK TO DETERMINE THE CURRENT STATUS OF A TRANSFER, AND LENGTH TO PROVIDE THE LENGTH IN BYTES OF THE LAST COMPLETED READ BY BUFFEI (INCLUDING TERMINAL CR LF). THESE FUNCTIONS ARE REFERENCED AS FOLLOWS:

```
M = IOCHEK(IUN)
L = LENGTH(IUN)
```

WHERE

IUN - THE LOGICAL UNIT NUMBER FOR WHICH BUFFEI OR BUFFEO WAS CALLED.

IOCHEK - AN INTEGER FUNCTION VALUE OF:
1 - FOR I/O STILL IN PROGRESS
2 - FOR I/O COMPLETE WITHOUT ERROR
3 - FOR I/O TERMINATED BY END-OF-FILE.
4 - FOR I/O TERMINATED BY ERROR

LENGTH - THE LENGTH IN BYTES OF THE READ DONE BY BUFFEI ON THIS UNIT. SHOULD BE CALLED ONLY AFTER AN IOCHEK CALL RETURNS A VALUE OF 2, FOR NORMAL COMPLETION.

+ NOTE

TO GET THE NUMBER OF ARRAY ELEMENTS, RATHER THAN BYTES, THE LENGTH RETURNED BY LENGTH SHOULD BE DIVIDED BY THE SAME VARIABLE USED AS NBYT IN THE CALL TO BUFFEI. HOWEVER, IF AN INTEGER ARRAY WAS USED WITHOUT THE /ON SWITCH FOR THE COMPILER, THE RESULT WILL BE TWICE THE DESIRED RESULT.

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

DEC PDP-11
DEC DOS/BATCH 9-2GC

DESCRIPTION

ALLD IS A PROGRAM TO COMPUTE MOLECULAR GEOMETRY, WRITTEN BY H. L. CARRELL OF THE INSTITUTE FOR CANCER RESEARCH. EACH OF THE MAJOR GEOMETRY CALCULATIONS IS PROVIDED BY A SEPARATE OVERLAY, WHICH MAY BE CALLED IN ANY ORDER.

PURPOSE

CALCULATES DISTANCES, ANGLES, TORSION ANGLES, PLANES.

LIMITATIONS

100 ATOMIC COORDINATES
48 SYMMETRY OPERATIONS
50 ATOMS IN LEAST SQUARES PLANES

SWITCH SETTINGS

2 UP - INPUT VIA UNIT 1 AND TTY
2 DOWN - INPUT VIA UNIT 1 ONLY
0 UP - SHORT OUTPUT

LOGICAL UNITS

1	PARAMETERS FOR NPAR (DEFAULT CR:)
6	OTHER INPUT (DEFAULT KB:)
	SWITCH 2 MUST BE UP
5	OUTPUT (DEFAULT LP:)

NOTE

IN ORDER TO ALLOW INPUT (IN ADDITION TO COORDINATES) TO BE EXTENDED VIA THE CR:

1. LOAD ALL CARDS IN CR:
2. SWITCHES 2 AND 0 MUST BE UP
3. RUN ALLD
4. AS COORDINATES ARE BEING READ IN,
   FLIP SWITCH 2 DOWN
5. SOLE INPUT IS NOW CR:
6. TO REACTIVATE KB: AS INPUT DEVICE,
   FLIP SWITCH 2 BACK UP DURING
   THE TYPING OF THE KB: MESSAGE
   WHICH INDICATES THE COMPLETION
   OF A ROUTINE

E.G. TO REACTIVATE KB: FOR CALCULATION OF PLANES, FLIP SWITCH 2 UP DURING THE TYPING OF ≠TORSION ANGLES COMPLETED≠. INPUT DEVICE IS THEN KB:.

INTRODUCTION

THIS IS A PROGRAM TO CALCULATE MOLECULAR GEOMETRY (DISTANCES, ANGLES, TORSION ANGLES AND LEAST SQUARES PLANES) ON THE PDP-11. THE PROGRAM CONSIST OF THE MAIN CALLING ROUTINE AND 5 OVERLAY ROUTINES. THESE ARE:

ROUTINE	FUNCTION
ALLD	MAIN CALLING ROUTINE
NPAR	PARAMETER INPUT
DIST	DISTANCE CALCULATION + BOND ANGLES
ANGL	BOND ANGLE CALCULATION
TORSN	TORSION ANGLE CALCULATION
PLANES	LEAST SQUARES PLANES

ANY ONE OF THE ROUTINES MAY BE CALLED FROM THE RESIDENT PROGRAM (ALLD). NPAR IS ALWAYS CALLED FIRST IN ORDER TO LOAD THE NECESSARY PARAMETERS (TITLE, CALL DIMENSIONS, SYMMETRY INFORMATION, ATOMIC COORDINATES AND ESD↑S). AFTER PARAMETER LOADING IS COMPLETE, ANY OF THE ROUTINES MAY BE CALLED IN ANY ORDER.

A BRIEF DESCRIPTION OF EACH OF THE ROUTINES IS GIVEN BELOW.

ALLD - THIS ROUTINE IS CORE RESIDENT AND SERVES ONLY TO CALL IN THE REQUESTED MOLECULAR GEOMETRY ROUTINES. THE INPUT TO THIS ROUTINE MAY COME FROM FORTRAN LOGICAL UNIT 1 (CR:) OR FROM 6 (KB:).

NPAR - PARAMETER INPUT ROUTINE. THE PURPOSE OF THIS ROUTINE IS TO LOAD THE NECESSARY PARAMETERS FOR THE CALCULATION OF THE MOLECULAR GEOMETRY. THE INPUT TO THIS ROUTINE MAY ONLY COME

FROM FORTRAN LOGICAL UNIT 1 (CR:).

DIST - CALCULATION OF INTERATOMIC DISTANCES AND ANGLES WITHIN A GIVEN RADIUS. UP TO 124 ADJACENT CELLS ARE SEARCHES. INPUT VIA LOGICAL UNIT 1 (CR:) OR 6 (KB:).

ANGL - CALCULATION OF BOND ANGLES AS SPECIFIED AT INPUT. EACH BOND ANGLE DESIRED MUST BE REQUESTED SEPARATELY. INPUT VIA UNIT 1 (CR:) OR 6 (KB:).

TORSN - CALCULATION OF TORSION ANGLES AS SPECIFIED BY INPUT. EACH TORSION ANGLE DESIRED MUST BE SPECIFIED. INPUT VIA UNIT 1 (CR:) OR 5 (KB:).

PLANES - LEAST SQUARES PLANE CALCULATION. THE ATOMS USED TO DEFINE THE PLANE ARE SPECIFIED AT INPUT TIME. IN ADDITION, THE COORDINATES OF ALL THE ATOMS FOR A GIVEN STRUCTURE RELATIVE TO THE PLANE MAY BE CALCULATED. INPUT VIA UNIT 1 (CR:) OR 6 (KB:).

INPUT DATA DESCRIPTION

THE INPUT TO ALLD MAY COME FROM THE KEYBOARD, OR FROM SOME DEVICE ASSIGNED TO UNIT 1, AS DETERMINED BY SWITCH 2. SOME OF THE DATA INPUT FORMATS ARE DIFFERENT, DEPENDING ON WHICH FORM OF INPUT IS SELECTED. THE USER MAY CATCH THE PROGRAM AT THE RIGHT TIME, I.E. AFTER AN OVERLAY HAS READ ALL ITS DATA, BUT BEFORE IT HAS FINISHED TYPING ITS COMPLETION LINE, TO GET ALLD TO REVERT TO KEYBOARD INPUT AFTER RUNNING FROM CARDS. IN ANY CASE, INPUT TO ALLD CONSISTS OF GROUPS OF DATA FOR THE SELECTED OVERLAYS. THE FIRST CARD OF EACH GROUP SELECTS THE OVERLAY. THE OVERLAY NPAR MUST BE EXECUTED FIRST, AND A SECOND ATTEMPT TO EXECUTE IT WILL TERMINATE THE PROGRAM. THE FIRST CARD OF EACH GROUP IS ACTUALLY READ BY THE MAIN ROUTINE, ALLD. THIS CARD, OR LINE FROM THE KEYBOARD, IS OF THE FORM

```
NOUT,NCALL
     (2I2) IF SWITCH 2 DOWN, READ FROM UNIT 1
     (I2,I1) IF SWITCH 2 UP, READ FROM UNIT 6
NOUT - OUTPUT UNIT NUMBER, MUST BE 5
NCALL - ROUTINE NUMBER
     0 - PARAMETER INPUT (NPAR)
          FORCES EXIT WHEN USED AGAIN
     1 - DISTANCES (DIST) AND BOND ANGLES (ANGL)
     2 - BOND ANGLES (ANGL)
     3 - TORSION ANGLES (TORSN)
     4 - LEAST SQUARES PLANES (PLANES)
```

INPUT TO NPAR

0. OVERLAY SELECTION CARD

```
NOUT, NCALL
     (2I2) IF SWITCH 2 DOWN, READ FROM UNIT 1
```

```
                (I2,I1) IF SWITCH 2 UP, READ FROM UNIT 6
            NOUT GIVES THE OUTPUT UNIT NUMBER, MUST BE 05
            NCALL MUST BE ZERO.
                E.G. 0500
```

THE FOLLOWING DATA SHOULD BE SET UP IN ADVANCE OF RUN ON CARDS DECK, OR TAPE DEPENDING ON FILE ASSIGNMENT FOR UNIT 1

```
1.  TITLE (60 ALPHANUMERIC CHARACTERS) (10A6)

2.  A,B,C, ALPHA, BETA, GAMMA, NTYP, NFMT, (6F10.5,2I2)
      CELL PARAMETERS
            A, B, C IN ANGSTROMS.
            ALPHA, BETA, GAMMA IN DEGREES.
            NTYP = 1      UCLALS4 FORMAT FOR COORDINATES
                ATOM LABEL LAST ON CARD
                UCLALS4 FORMAT (3F10.5, 40X, A6) X,Y, Z, LABEL
            NTYP = 2      XRAY FORMAT FOR COORDINATES
                ATOM LABEL FIRST ON CARD
                XRAY FORMAT (7X, A6, 3F8.4) LABEL, X,Y,Z
            NFMT = 0 FIXED FORMAT
            NFMT = 1 VARIABLE FORMAT
                FORMAT SPECIFICATION CARD MUST BE INCLUDED

3. NATOM, NEQ, NCEN, NSIG  (4I3)
            NATOM - NO. OF ATOMS TO BE INPUT (MAX = 100)
            NEQ   - NO. OF SYMMETRY EQUIVALENT POSITIONS TO BE READ.
            NCEN  - 0 NO CENTER OF SYMMETRY IMPLIED AT THE ORIGIN
                  - 1 CENTER OF SYMMETRY IMPLIED AT THE ORIGIN
                  POSITIONS RELATED BY IT WILL BE GENERATED.
            NSIG FLAGS INPUT OF ESTIMATED STANDARD DEVIATIONS.
                  NSIG=0, NO ESD↑S TO BE INPUT
                  NSIG=1, ESD↑S TO BE INPUT
```

NOTE: ALLD DOES NOT TREAT CELL CENTERING (A,B,C,F,I) EG: FOR SPACE GROUP C2, ALL 4 CARDS MUST BE PUNCHED.

4. SYMMETRY INFORMATION CARDS (NEQ CARDS OF THIS TYPE) FORMAT (30 A1)

COLS 1-30 SYMMETRY INFORMATION. ONE EQUIVALENT POSITION PER CARD. THE GENERAL EQUIVALENT INFORMATION FOUND IN THE INTERNATIONAL TABLES IS SUFFICIENT AND SHOULD BE PUNCHED VERBATIM. IN THE CASE OF A CELL WHICH IS A,B,C,I OR F CENTERED, IT IS NECESSARY THAT ALL POSITIONS ARISING FROM THE CENTERING CONDITIONS BE EXPLICITLY PUNCHED.

NOTE...IF THE CELL HAS BEEN CODED AS CENTROSYMMETRIC (NCEN = 1), DO NOT PUNCH THOSE POSITIONS RELATED TO THE GENERAL SET BY THE CENTER AT THE ORIGIN.

NOTE...THE READING OF INFORMATION ON ANY GIVEN CARD ***MUST*** BE TERMINATED BY A PERIOD.

E.G....FOR SPACE GROUP P21 (B AXIS UNIQUE), NEQ= 2. THE FOLLOWING 2 CARDS WOULD BE REQUIRED (PUNCHED STARTING IN COLUMN 1):

X, Y, Z

-X,1/2+Y,-Z.

5. FORMAT CARD IF NFMT = 1

6. COORDINATE CARDS

```
      FOR NFORM = 1:  (UCLALS4)  FORMAT (3F10.5,40X,A6)
          COLS  1-10 X COORDINATE IN CELL FRACTION
          COLS 11-20 Y COORDINATE IN CELL FRACTION
          COLS 21-30 Z COORDINATE IN CELL FRACTION
          COLS 71-76   ATOM IDENTIFICATION
      FOR NFORM = 2:  (XRAY70) FORMAT (7X,A6,3F8.4)
          COLS  8-13   ATOM IDENTIFICATION
          COLS 14-21 X COORDINATE IN CELL FRACTIONS
          COLS 22-29 Y COORDINATE IN CELL FRACTIONS
          COLS 30-37 Z COORDINATE IN CELL FRACTIONS
```

7. ESD'S FOR THE NATOM COORDINATES

THESE CARDS ARE INCLUDED ONLY IF NSIG = 1. NO ATOM IDENTIFICATION IS READ SO THAT THEY MUST HAVE THE SAME INPUT ORDER AS THE COORDINATE CARDS.

```
      FORMAT(3F10.5)
          COLS  1-10  ESD OF X
          COLS 11-20  EDS OF Y
          COLS 21-30  ESD OF Z
```

INPUT TO DIST AND ANGL

0. OVERLAY SELECTION CARD

```
          NOUT, NCALL
               (2I2) IF SWITCH 2 DOWN, READ FROM UNIT 1
               (I2,I1) IF SWITCH 2 UP, READ FROM UNIT 6
          NOUT MUST BE 5
          NCALL MUST BE 1
```

DIST: AND ANGL: REQUIRES 1 LINE OF INPUT EITHER ON KB: OR CR:
NOR1, NOR2, NTAR1, NTAR2, NAI, NAJ, NBI NBJ, NCI, NCJ, DMAX, DBOND

NOR1 THROUGH NOR2 INCLUSIVE DEFINE THE ORIGIN ATOMS ABOUT WHICH THE DIS- TANCES WITHIN A RADIUS OF DMAX ANGSTROMS ARE TO BE COMPUTED.

NTAR1 THROUGH NTAR2 INCLUSIVE DEFINE THE TARGET ATOMS TO BE SEARCHED TO DETERMINE IF ANY OF ATOMS NTAR1 THROUGH NTAR ARE WITHIN DMAX ANGSTROMS OF NOR1 THROUGH NOR2.

NAI, NAJ ARE THE MINIMUM AND MAXIMUM NUMBER OF TRANSLATIONS ALONG THE ≠A≠ AXIS INCLUDED IN THE DISTANCE SEARCH.

NBI, NBJ, NCI, NCJ APPLY TO THE ≠B≠ AND ≠C≠ DIRECTIONS RESPECTIVELY. IN MOST INSTANCES A 27 CELL SEARCH DEFINED BY -1,1,-1,1,-1,1 FOR THE THREE CELL DIRECTIONS WILL BE MORE THAN SUFFIEIENT FOR FINDING ALL DISTANCES WITHIN THE DMAX RADIUS. THE SMALLER THE VOLUME FOR THE SEARCH, THE FASTER THE CALCULATION WILL BE COMPLETED.

DMAX IS THE MAXIMUM DISTANCE FOR THE SEARCH.

THE BOND ANGLE CALCULATION ROUTINE CONSISTS OF ALLOWING NOR1 THROUGH NOR2 INCLUSIVE TO SUCCESSIVELY SERVE AS THE VERTEX OF A 3 ATOM BOND ANGLE CALCULATION. THE 2 END ATOMS ARE CHOSEN FROM NTAR1 THROUGH NTAR2 INCLUSIVE WITH THE RESTRICTION THAT THE 3 ATOMS IN EACH ANGLE CAN OCCUPY AT MOST 2 UNIQUE SYMMETRY EQUIVALENT POSITIONS AND THAT DMAX IS THE MAXIMUM DISTANCE BETWEEN THE VERTEX ATOM AND ITS ENDPOINT ATOMS.

INPUT TO ANGL

0. OVERLAY SELECTION CARD
NOUT, NCALL
(2I2) IF SWITCH 2 DOWN, READ FROM UNIT 1
(I2,I1) IF SWITCH 2 UP, READ FROM UNIT 6
NOUT MUST BE 5
NCALL MUST BE 2

ANGL: EACH ANGLE DESIRED MUST BE SPECIFIED INDIVIDUALLY.

FOR INPUT FROM UNIT 1.
BOND ANGLE CODE CARDS (15I3) SWITCH 2 IS DOWN

COLS	1-2	TRANSLATION ALONG A AXIS FOR ATOM 1
COLS	3-4	TRANSLATION ALONG B AXIS FOR ATOM 1
COLS	5-6	TRANSLATION ALONG C AXIS FOR ATOM 1
COLS	7-8	EQUIVALENT POSITION NUMBER FOR ATOM 1
COLS	9-10	ATOM NUMBER FROM INPUT ATOMS FOR ATOM 1
COLS	11-12	TRANSLATION ALONG A AXIS FOR ATOM 2
COLS	13-14	TRANSLATION ALONG B AXIS FOR ATOM 2
COLS	15-16	TRANSLATION ALONG C AXIS FOR ATOM 2
COLS	17-18	EQUIVALENT POSITION NUMBER FOR ATOM 2
COLS	19-20	ATOM NUMBER FROM INPUT LIST FOR ATOM 2
COLS	21-22	TRANSLATION ALONG A AXIS FOR ATOM 3
COLS	23-24	TRANSLATION ALONG B AXIS FOR ATOM 3
COLS	25-26	TRANSLATION ALONG C AXIS FOR ATOM 3
COLS	27-28	EQUIVALENT POSITION NUMBER FOR ATOM 3
COLS	29-30	ATOM NUMBER FROM INPUT LIST FOR ATOM 3

THE ANGLE CALCULATION IS TERMINATED BY -1 PUNCHED IN COLS 9-10

FOR TELETYPE INPUT:

FOR TELETYPE INPUT THE ATOM NUMBERS ARE INPUT FIRST FOLLOWED BY THE SYMMETRY CODE FOR THE ATOMS: NA1, NA2, NA3, NA(1), NB(1), NC(1), NEQ(1), NA(2), NB(2), NC(2), NEQ(2), NA(3), NB(3), NC(3), NEQ(3)

IF THE EQUIVALENT POSITION NUMBER IS ≠0≠ IT IS ASSUMED TO BE ≠1≠ THUS IF THE ATOMS IN THE ANGLE CALCULATION ARE IN 1 MOLECULE IN THE SAME ASYMMETRIC UNIT, ONLY THE ATOM NUMBERS NEED TO BE SPECIFIED. THE ANGLE IS FOR NA1-NA2-NA3. THE TELETYPE LINE OF INPUT MUST BE TERMINATED BY A COMMA ≠,≠ AND CARRIAGE RETURN.

INPUT TO TORSN

0. OVERLAY SELECTION CARD
NOUT, NCALL
(2I2) IF SWITCH 2 DOWN, READ FROM UNIT 1
(I2,I1) IF SWITCH 2 UP, READ FROM UNIT 6
NOUT MUST BE 5
NCALL MUST BE 3

TORSN: TORSION ANGLES WITH E.S.D.'S

FOR INPUT FROM UNIT 1:
TORSION ANGLE CODE CARDS. 4 ATOMS PER ANGLE SWITCH 2 DOWN.
FORMAT(20I2)

COLS	1-2	TRANSLATION ALONG A AXIS FOR ATOM 1
COLS	3-4	TRANSLATION ALONG B AXIS FOR ATOM 1
COLS	5-6	TRANSLATION ALONG C AXIS FOR ATOM 1
COLS	7-8	EQUIVALENT POSITION NUMBER FOR ATOM 1
COLS	9-10	ATOM NUMBER FROM INPUT LIST FOR ATOM 1
COLS	11-20	CODE WORDS FOR ATOM 2
COLS	21-30	CODE WORDS FOR ATOM 3
COLS	21-30	CODE WORDS FOR ATOM 4

THE TORSION ANGLE CALCULATION IS TERMINATED BY PUNCHING -1 IN COLUMNS 9 AND 10

FOR INPUT FROM UNIT 6:

TELETYPE INPUT IS SIMILAR TO THAT FOR BOND ANGLES EXCEPT THAT 4 ATOM CODE SPECIFICATIONS ARE NECESSARY. TERMINATE LINE WITH COMMA AND CARRIAGE RETURN. THE TORSION ANGLE 1-2-3/2-3-4 IS CALCULATED.

INPUT TO PLANES

0. OVERLAY SELECTION CARD
NOUT, NCALL
(2I2) IF SWITCH 2 DOWN, READ FROM UNIT 1
(2I,I1) IF SWITCH 2 UP, READ FROM UNIT 6
NOUT MUST BE 5
NCALL MUST BE 4

PLANES: LEAST SQUARES PLANES

CALCULATES THE EQUATION OF THE PLANE DEFINED BY THE USER. UP TO 50 ATOMS MAY DEFINE THE PLANE. THE PROGRAM WILL THEN COMPUTE THE COORDINATES OF THE ENTIRE ATOM ARRAY WITH RESPECT TO THE PLANE FOR AS MANY SYMMETRY CODE SETS AS DESIRED.

FOR INPUT FROM UNIT 1:

1 — NUMBER OF ATOMS IN PLANE, SUBTITLE FOR CALCULATION (I5,10A4)

NAP, (TITLE(I),I=1,10)
COLS 1-5 NUMBER OF ATOMS TO BE INCLUDED IN THIS CALCULATION- ONLY USED TO CALCULATE PLANE MAX=50.
COLS 6-45 SUBTITLE FOR THIS PARTICULAR LEAST SQUARES PLANE
THE LEAST SQUARES PLANES CALCULATION IS TERMINATED BY A -1 PUNCHED IN COLS 4 AND 5 OF THIS CARD

2. ATOM SPECIFICATIONS FORMAT(5(5I3))

SPECIFICATIONS FOR 5 ATOMS ARE PUNCHED ON THESE CARDS SO THAT NAP/5 CARDS ARE NECESSARY IF NAP=0(MODULO 5) OR NAP/5+1 IF NAP=0(MODULO5)
COLS 1-3 TRANSLATION ALONG A AXIS FOR ATOM 1
COLS 4-6 TRANSLATION ALONG B AXIS FOR ATOM 1
COLS 7-9 TRANSLATION ALONG C AXIS FOR ATOM 1
COLS 10-12 EQUIVALENT POSITION NUMBER FOR ATOM 1
COLS 13-15 ATOM NUMBER FROM INPUT LIST FOR ATOM 1

3. SYMMETRY CODE CARD FOR TRANSFORMATION OF COORDINATES TO THE AXIAL SYSTEM WHICH DESCRIBES THE PLANE. THIS IS USEFUL IF THE USER WANTS THE RELATION OF THE ATOMS NOT INCLUDED IN THE PLANE WITH RESPECT TO THE PLANE. NA,NB,NC,NE (4I4). READING OF SYMMETRY CODE CARDS TERMINATED BY A CARD WITH ≠-1≠ IN COL 15 AND 16
EG: 0001 THEN ALL INPUT PRINTED OUT

FOR INPUT FROM UNIT 6:

1. SUBTITLE OF A PLANE (15A4).

2. ATOM SPECIFICATION (5I5)

1 LINE PER ATOM. EACH LINE CONSISTS OF: ATOM NUMBER, A TRANSLATION, B TRANSLATION, C TRANSLATION, EQUIVALENT POSITION NUMBER END OF LIST IS DENOTED BY ATOM NUMBER OF < 0 IF ATOM NUMBER ONLY IS INPUT, THE SYMMETRY POSITION 0,0,0,1 IS ASSUMED.

3. SAME AS 3 ABOVE, TO TERMINATE READING OF THESE CARDS, SIMPLY BIT (CR) PLANE CODE, BUT IN THE REMAINDER OF THE INPUT ATOM LIST. A COMMA MUST COME AFTER THE EQUIVALENT POSITION NUMBER.

NOTE: KB: INPUT IS MUCH FASTER THAN TYPING ALL THE CARDS NEEDED FOR CR: INPUT.

```
SAMPLE RUN

S*RU ALLD

PARAMETER INPUT COMPLETE
NOUT,NCALL..*5,1

CALCULATE ANGLES(BLANK=YES)*

PRINT DISTANCES(BLANK=YES)*

ENTER  NOR1, NOR2, NTAR1,NTAR2,NAI,NAJ,NBI,NBJ,NCI,NCJ,DMAX,DBOND
*1,5,1,5,-1,1,-1,1,-1,1,2.0,2.0

CALCULATE ANGLES(BLANK=YES)*NO

PRINT DISTANCES(BLANK=YES)*NO

ENTER  NOR1 ,NOR2,  NTAR1,NTAR2,NAI,NAJ,NBI,NBJ,NCI,NCJ,DMAX,DBOND
*

DISTANCE CALCULATION COMPLETE

NOUT,NCALL..*5,2

ANGLE CODE...*1,2,3,

ANGLE CODE...*4,5,6,0,0,0,1,0,0,0,2,0,0,0,1,

ANGLE CODE...*

ANGLE CALCULATION COMPLETE..

NOUT,NCALL..*5,3

TORSION ANGLE CODE..*1,2,3,4,

TORSION ANGLE CODE..*5,6,7,8,0,0,0,2,0,0,0,2,0,0,0,2,0,0,0,2,

TORSION ANGLE CODE..*

TORSION ANGLES COMPLETED..
NOUT,NCALL..*5,4

TELETYPE INPUT
SUBTITLE...*SGG PLANE OF ATOMS E1,2,3,4,5

SYMMETRY CODE FOR THE ATOMS IN CALCULATION
*1,
*2,
*3,
*4,
*5,
*

SYMMETRY CODE...NA,NB,NC,NE..
```

```
*0,0,0,1

THE EQUIVALENT POSITION NO.(NE) IS TOO LARGE.
REENTER CODE..TERMINATE THE INPUT WITH A COMMA.

SYMMETRY CODE...NA,NB,NC,NE..
*0,0,0,1,

SYMMETRY CODE...NA,NB,NC,NE..
*

TELETYPE INPUT
SUBTITLE...*

SYMMETRY CODE FOR THE ATOMS IN CALCULATION
*

NOUT,NCALL..*5,0

END OF RUN.....
```

01-JUL-75

AUTHOR: H. L. CARRELL

CALCSF - 03/18/76

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

DEC PDP-11
DEC DOS/BATCH 9-20C

DESCRIPTION

CALCSF IS A PROGRAM TO COMPUTE STRUCTURE FACTORS, WRITTEN BY H. L. CARRELL OF THE INSTITUTE FOR CANCER RESEARCH.

PURPOSE

CALCULATES STRUCTURE FACTORS

LIMITATIONS

24 EQUIVALENT POSITIONS
100 ISOTROPIC ATOMS OR A NUMBER OF ATOMS DETERMINED BY
NISO + 2*NAN = 100
NISO = NUMBER OF ISOTROPIC ATOMS
NAN = NUMBER OF ANISOTROPIC ATOMS

LOGICAL UNITS

1	INPUT OTHER THAN REFLECTION DATA (DEFAULT CR:)
7	REFLECTION DATA FROM MSRED (DEFAULT SY:HKLDAT.DAT)
5	PRINTED OUTPUT (DEFAULT LP:)
4	OUTPUT TO FOURIER PROG (DEFAULT SY:FOURR.DAT)

FILE ASSIGNMENTS

1 MUST BE ASSIGNED IF OTHER THAN CR:

NB: IF IT IS DESIRED TO RUN A FOURIER SYNTHESIS IMMEDIATELY AFTER RUNNING CALCSF, IT IS NECESSARY TO DE-ASSIGN THE FILES BY:

FI

AND THEN LOG IN AGAIN.

CALCSF - 03/18/76

INPUT

THE INPUT TAPE (LOGICAL UNIT 7) MUST BE A NON-FORMATTED, BINARY FILE WITH THE FOLLOWING INFORMATION FOR EACH REFLECTION:

H,K,L,NOTIN, FOBS, SIGMAF, SINL, F(1)....F(10), WHERE NOTIN INDICATES OBSERVED (=0) OR UNOBSERVED (=1) FOBS,SIGMAF ARE THE OBSERVED STRUCTURE AMPLITUDE AND ITS ESD. F(1)...F(10) ARE FORM FACTORS FOR 1 TO 10 ATOMS, AS WRITTEN BY THE DATA REDUCTION PROGRAM MSRED

CARD READER: CONTROL INFORMATION

OUTPUT

PRINTER: SEE ATTACHED EXAMPLE.

DISC: (OPTIONAL) (FOURR.DAT)-A NON-FORMATTED BINARY FILE FOR INPUT TO THE FOURIER SYNTHESIS PROGRAM. EACH RECORD CONTAINS H,K,L,NOTIN,(FO), (FC), (FO-FC), ALPHA

INPUT CARDS

THE FOLLOWING INPUT DATA MUST BE SUPPLIED BY THE USER AT EXECUTION TIME.

1. FILE ASSIGNMENT (12A2) FILENAME OF INPUT DATA FILE
EXAMPLE - MT0:JUNK
THIS CARD IS NOT USED IN OLDER VERSIONS OF CALCSF.

2. TITLE CARD (15A4)

3. NSF,NEQV,NCENT,LAT,NSUPP,NFOURR,NEMAP(3I5,4X,A1,3I5)
NSF - NUMBER OF ATOMS TO BE INPUT
NEQV - NUMBER OF SYMMETRY EQUIVALENT POSITIONS NOT RELATED BY A CENTER OF SYMMETRY AT THE ORIGIN NOR BY LATTICE TRANSLATIONS AS I, B, ETC. MARGINS 0,0
NCENT (0)/(1) ... (ACENTRIC)/(CENTRIC)
LAT P,B,A,C,F OR I
NSUPP (0)/(1)/(2)/(3) ... (DO NOT LIST REFLECTION DATA)/(LIST ALL DATA)/(LIST OBSERVED DATA ONLY)/ (LIST UNOBSERVED DATA ONLY)
NFOURR (0)/(1) (DO NO WRITE FOURIER FILE)/(DO WRITE FOURIER FILE) THIS FILE CONTAINS H,K,L,NOTIN,/FO/,/FC/,//FO/-/FC//,ALPHA FOR EACH REFLECTION.

4. SCALE,SLMIN,SIMAX,WTMIN,BCRYST(5F10.6)
SCALE - SCALE FACTOR FOR FOBS
SLMIN - MINIMUM SINE / FOR CALCULATION OF E'S
SLMAX - MAXIMUM SINE / FOR CALCULATION IF SLMAX < 0. THEN ALL DATA WITH SINL > SLMIN WILL BE USED.
WTMIN - MINIMUM WEIGHT OF REFLECTION TO BE WRITTEN TO FOURIER FILE. IF WTMIN =0.0 THEN ALL OBSERVED DATA WILL BE GIVEN W = 1.0. IF NEMAP = 1 THEN ONLY DATA WITH E > WTMIN WILL BE USED.
BCRYST - OVERALL TEMPERATURE FACTOR TO BE USED IN CALCULATING E VALUES. (IF TEMPERATURE FACTORS ARE 0.0, BCRYST WILL BE USED AS THE ISOTROPIC TEMPERATURE FACTOR.)

5. FDP(10),FDPP(10) (2 CARDS) 2(10 F6.2)
ONE CARD WITH FDP FOR UP TO 10 ATOMS
DELTA F' - REAL COMPONET OF ANOMALOUS SCATTERING FOR ATOM TYPE - SAME ORDER AS FORM FACTOR CURVES WERE INPUT.
ONE CARD WITH FDPP
DELTA F" - IMAGINARY
USE BLANK CARDS IF THERE IS NO ANOMALOUS SCATTERING.

6. EPS (7) (7F5.0)
EPSILON VALUES TO CALCULATE E'S FOR THE SEVEN CLASSES OF REFLECTIONS:
HKL,HK0,H0L,0KL,H00,0K0,00L. THESE CAN BE TAKEN AS THE THEORETICAL VALUES OR AS THOSE REFINED BY SCALER (WILSON PLOT). USE BLANK CARD FOR STRUCTURE FACTOR CALCULATION.

7. WGP (8) (8F5.0)
THE PARITY GROUP WEIGHTS FOR THE EIGHT PARITY CLASSES OF REFLECTIONS:
GGG,GGU,GUG,GUU,UGG,UGU,UUG,UUU. AGAIN THESE CAN BE THEORETICAL OR COME FROM SCALER. USE BLANK CARD FOR STRUCTURE FACTOR CALCULATION.

8. THE NUMBER OF EACH TYPE OF ATOM UP TO 10 TYPES. FNA(10) (10F5.0)
BLANK CARD FOR STRUCTURE FACTOR CALCULATION.

9. SYMMETRY EQUIVALENT POSITIONS (30A1)
1 CARD FOR EACH OF THE NEQV POSITIONS. THESE ARE PUNCHED AS GIVEN IN THE INTERNATIONAL TABLES, E.G. X,Y,Z - X,Y,Z, ETC.

10. NXYZ,XTEM (I5,F10.2)
NXYZ (1)/(2) ... (ATOM LABEL LAST ON COORDINATE CARD)/(ATOM LABEL FIRST ON COORDINATE CARD) USE 1 FOR LINUS OUTPUT, 2 FOR FMLS OUTPUT.
XTEM FACTOR BY WHICH B12, B13, B23 ARE TO BE MULTIPLIED SO THAT THE ANISOTROPIC TEMPERATURE FACTORS CONFORM TO THE FOLLOWING EQUATION FOR THE TEMPERATURE FACTOR
EXP(-H*H*B11-K*K*B22-L*L*B33-H*K*B12-H*L*B13-K*L*B23)

11. FMT (15A4)
FORMAT OF COORDINATE CARDS
SEE DESCRIPTION OF CARD 13.

12. FMTA (15A4)

FORMAT OF TEMPERATURE FACTOR CARDS FOR ANISOTROPIC TEMPERATURE FACTORS. (SEE DESCRIPTION OF CARD 13). USE A BLANK CARD HERE IF TEMPERATURE FACTORS ARE ISOTROPIC AND B ON ATOM CARD 0.0

13.1 COORDINATE CARDS X,Y,Z,B,G,ITBL,ATOM LABEL OR ATOM LABEL,X,Y,Z,B,G, ITBL, AS DETERMINED BY CARD 9 (NXYZ).

X,Y,Z THE FRACTIONAL ATOMIC COORDINATES FOR EACH ATOM.

B ISOTROPIC TEMPERATURE FACTOR. IF THIS IS 0.0 OR BLANK THEN CARD 12.2 WILL BE READ.

G THE OCCUPANCY FACTOR (USUALLY 1.0 UNLESS THE ATOM OCCUPIES A SPECIAL POSITION).

ITBL NUMBER OF THE FORM FACTOR FOR THIS ATOM. IF THE ATOM IS A CARBON ATOM AND THE FORM FACTOR FOR CARBON IS THE FIRST, THEN ITBL - 1.

13.2 TEMPERATURE FACTOR CARDS B11,B22,B33,B12,B13,B23 (ANISOTROPIC TEMPERATURE PARAM.) IF B22 IS LESS THAN OR EQUAL TO 0, THEN B11 WILL BE TAKEN AS THE ISOTROPIC TEMPERATURE FACTOR.

RESTRICTIONS

1) 24 UNIQUE EQUIVALENT POSITIONS

2) 100 ISOTROPIC ATOMS OR A NUMBER OF ATOMS DETERMINED BY THE RELATIONSHIP NISO+2*NAN=100, WHERE NISO= NUMBER OF ISOTROPIC ATOMS. NAN = NUMBER OF ANISOTROPIC ATOMS.

THE INPUT TAPE (LOGICAL UNIT 7) MUST BE A NON-FORMATTED, BINARY FILE WITH THE FOLLOWING INFORMATION FOR EACH REFLECTION:

H,K,L,NOTIN,FOBS,SIGMAF,SINL,F(1)...F(10), WHERE NOTIN INDICATES OBSERVED (=0) OR UNOBSERVED (=1) FOBS,SIGMAF ARE THE OBSERVED STRUCTURE AMPLITUDE AND ITS ESD. F(1)...F(10) ARE FORM FACTORS FOR 1 TO 10 ATOMS.

THIS FILE MAY BE WRITTEN AT DATA REDUCTION

CALCSF - 03/18/76

SAMPLE RUN

CARD INPUT

```
MT0:EDCIT.DAT
ETHYLENEDIAMINE  CITRATE
17    1    1    P    0    1    0    1 .040      0.0       0.7       0.0
 2.2 14.   4.  16.
X,Y,Z
    2
(7X,A4,2X,3F8.5,F7.3,F8,5,I3)
ATOM      1     0.57780 0.17060 0.16360  2.2       1.0       1
ATOM      2     0.57590 0.45170 0.29250  2.2       1.0       1
ATOM      3     0.80540 0.52930 0.30750  2.2       1.0       1
ATOM      5     0.76270 0.00750 0.27730  2.2       1.0       1
ATOM      6     0.61410 0.03880-0.33050  2.2       1.0       1
ATOM      7     0.57440 0.26320-0.22800  2.2       1.0       1
ATOM      8     0.29370 0.30640 -.07060  2.2       1.0       2
ATOM      9     0.69650 0.42870 0.27448  2.2       1.0       3
ATOM     10     0.36520 0.25970 0.37630  2.2       1.0       2
ATOM     11     0.98100 0.12660 0.54390  2.2       1.0       3
ATOM     14     0.71750 0.27360 0.22560  2.2       1.0       3
ATOM     15     0.64430 0.17500-0.19600  2.2       1.0       3
ATOM     16     0.85950 0.12440 0.41260  2.2       1.0       3
ATOM     17     0.77550 0.22420 0.02220  2.2       1.0       3
ATOM     19     0.83560 0.27640 0.43830  2.2       1.0       3
ATOM     21     0.21570 0.23340 0.20530  2.2       1.0       3
ATOM     22     0.21140 0.33650 0.09150  2.2       1.0       3
```

KB INPUT

```
RU CALCSF
STRUCTURE FACTOR CALCULATION
     5-METHYLCHRYSENE.
NSF=  31      NEQV=   2      NCENT=  1     LATTICE= P
SCALE FACTOR FOR FCALC=   1.000
THE LOWER AND UPPER LIMITS OF SIN(THETA)/LAMBDA ARE 0.000 AND 0.000
RESPECTIVELY
WTMIN=   0.000
B(OVERALL)=   0.00
EPSILON VALUES FOR THE REFLECTION ZONES
  HKL     0KL     H0L     HK0     H00     0K0     00L
  1.00    1.00    1.00    1.00    1.00    1.00    1.00
PARITY GROUP WEIGHTS
  GGG     GGU     GUG     GUU     UGG     UGU     UUG     UUU
  1.00    1.00    1.00    1.00    1.00    1.00    1.00    1.00
CELL CONTENTS AND ANOMALOUS SCATTERING VALUES.
ATOM TYPE     NO.       FOP       FOPP
INPUT EQUIVALENT POSITIONS.
  1      X,Y,Z
  2      -X,1/2+Y,1/2-Z
INPUT ATOMIC PARAMETERS
NO.  ATOM     X         Y         Z         G         B11       B22       B33       B12
B13
  1      1    0.3613    0.6981    0.0385    1.0000    8.150
  2      2    0.3424    0.5333   -0.0043    1.000     9.135
```

3	3	0.3740	0.4247	-0.0031	1.0000	10.250
4	5	0.5952	0.3237	0.1561	1.0000	6.278
5	6	0.6527	0.3246	0.2067	1.0000	8.706
6	7	0.7309	0.4838	0.3152	1.0000	10.214
7	8	0.7453	0.6398	0.3552	1.0000	9.174
8	9	0.7022	0.8159	0.3531	1.0000	8.510
9	10	0.6358	0.8315	0.3009	1.0000	7.167
10	11	0.5042	0.8553	0.1899	1.0000	7.989
11	12	0.4417	0.8643	0.1435	1.0000	9.901
12	13	0.4202	0.6759	0.0907	1.0000	7.149
13	14	0.4717	0.5067	0.0947	1.0000	4.986
14	15	0.5373	0.5059	0.1487	1.0000	6.623
15	16	0.5526	0.6580	0.1957	1.0000	6.239
16	17	0.6169	0.6705	0.2491	1.0000	5.878
17	18	0.6663	0.4728	0.2555	1.0000	7.711
18	19	0.5828	0.1364	0.1061	1.0000	9.883
19	2	0.0243	0.9149	0.0958	1.0000	7.630
20	3	0.0454	0.7396	0.0699	1.0000	5.576
21	4	0.0932	0.5583	0.1048	1.0000	9.375
22	5	0.1945	0.4737	0.3125	1.0000	5.760
23	7	0.1945	0.5437	0.4739	1.0000	6.896
24	8	0.1700	0.7240	0.4972	1.0000	8.742
25		0.1214	0.9103	0.4621	1.0000	1.957
26	11	0.0642	1.0089	0.2778	1.0000	5.774
27	13	0.0799	0.7917	0.1944	1.0000	7.428
28	14	0.1050	0.6099	0.1709	1.0000	9.188
29	17	0.1281	0.8007	0.3699	1.0000	8.608
30	18	0.1693	0.6197	0.3961	1.0000	8.455
31	19	0.2298	0.2910	0.3080	1.0000	8.845

```
 TIME    18:31:33
SCALE FACTOR FOR FOB =  0.23260     NSUPP=  0     NFCORR=  1
SLMIN=  0.0000          SLMAX=  0.0000          WTMIN=  0.0000
TOTAL NO. OF DATA = 2772     NO. UNOBSERVED = 1045
R(CONVENTIONAL)=     0.422          R(WEIGHTED)=      0.65692
2772 DATA WRITTEN ONTO THE FOURIER DATA FILE.
SUM/DLF/(OBS)= 10812.322 SUM/FOB/(OBS)= 25629.420  SUM/FCALC/(OBS)=
20827.623
SUM W*DLF*DLF = 367129.8125  SUM W*FO*FO = 850721.6250 SUM W*FC*FC=
686549.4375
SUM/DLF/(UNOB)= 3344.4514  SUM/FO/(UNOB)= 2272.1790 SUM/FC/(UNOB)=
3550.2039
R FACTORS FOR THE REFLECTION GROUPS(OBSERVED DATA ONLY)
GROUP       R       SUMFOBS      SUMDLF      SUMFC          NO.
HKL      0.421  0.1706E 05  0.7187E 04  0.1334E 05     1304
0KL      0.395  0.1428E 04  0.5640E 03  0.1346E 04      100
H0L      0.405  0.4892E 04  0.1982E 04  0.4548E 04      241
HK0      0.398  0.1098E 04  0.4370E 03  0.7026E 03       47
H00      0.694  0.5115E 03  0.3549E 03  0.3610E 03       15
0K0      0.825  0.2889E 02  0.2384E 02  0.8943E 01        2
00L      0.429  0.6134E 03  0.2634E 03  0.5178E 03       18
MAXH= 21  MAXK= 5  MAXL= 23  FOMAX= 252.73  FCMAX= 198.19  DFMAX= 114.63
H INDEX CHANGES  21 TIMES.
K INDEX CHANGES  108 TIMES.
```

01-JUL-75

CALCSF-7
AUTHOR: H. L. CARRELL

CALCSF - 03/18/76

TIME 18:47:42

"CART."

Program to compute cartesian coordinates relative to any given plane. The input consists of the crystal ccoordinates of the desired atoms, the symmetry equivalent positions, the transformation matrix, and the symmetry code cards for each calculation. The transformation matrix may be obtained from the least squares plane calculation in ALL D2 and the symmetry code cards from the distance calculation in ALL D2.

INPUT: XYZ,+-/123456

A. Title Card (cols 1-72)

B. NAT,NEQ,NTPY (3I5)
cols 1-5 NAT-# of atomic coordinate cards to be read
6-10 NEQ-# of sym. equiv. pos. cards to be read (including those related by a center of sym. at the origin)
15 NTYP-("0" or blank)/(1)-(UCLA COORES.)/(XRAY COORDS)

C. Equivalent Position Code Cards
cols 1-45 (4.5A1)
Punched as found in the International Tables (same as for ALL D2)
ex. cols 12345678910
x,y,z
1/2-x,y,z

D. Transformation Matrix Cards (3 cards) (4F15.7)
(T)(X)=(X')
where (T) is the transformation matrix
(X') the cartesian coordinates

E. Atomic Coordinate Cards
NAT cards in UCLA or XRAY format as specified by NTYP

F. Symmetry Operation for calculation of coordinates (4I3)

cols 1-3	# of translations in "a" direction	NA
4-6	# " " " "b" "	NB
7-9	#" " " "c" "	NC
10-12	equiv. pos. #	NE

as many "F" cards are used as calculations desired.

"CART." program usually takes less than 1 second of computer time

∴ 2 or more runs may be made back to back by placing a "-1" for NE in the last "F". card and following this card with all cards "A" through "F" for the next compound. CXQT ABC.CART IS NOT REPEATED FOR EACH ADDITIONAL CMPD.

CARTÉS

```
0001          REAL NAME
0002          DIMENSION A(3),B(3),C(3),D(3),T(12),TR(24,3),SS(3,3),RN(3)
             1S (24,3,3),X(100),Y(100),Z(100),NAME(100),IEQ(45)
0003          DIMENSION NEQ(14)
0004          COMMON NEQ
0005          READ(1,77)(NEQ(J),J=1,14)
0006       77 FORMAT(14A1)

A002 012620
$CO
0007      700 READ(1,1)(T(I),I=1,12)
0008        1 FORMAT(12A4)
0009          PRINT 101,(T(I),I=1,12)
0010      101 FORMAT(12A4)
0011          READ(1,2)NAT,NEQV,NTYP
0012        2 FORMAT(3I5)
0013          PRINT 102,NAT,NEQV
0014      102 FORMAT(1H0 I5,13H ATOMS INPUT.,5X,I5,22H EQUIVALENT POSIT
0015          PRINT 103
0016      103 FORMAT(28H0INPUT EQUIVALENT POSITIONS. /5H0 NO.    )
0017          DO 20 I=1,NEQV
0018          READ(1,3)(IEQ(J),J=1,45)
0019          PRINT 4,I,(IEQ(J),J=1,45)
0020          CALL EQPOS(IEQ,RN,SS)
0021        3 FORMAT(45A1)
0022        4 FORMAT(I5,4X,45A1)
0023          DO 19 J=1,3
0024          TR(I,J)=RN(J)
0025          DO 18 K=1,3
0026       18 S(I,J,K)=SS(J,K)
0027       19 CONTINUE
0028       20 CONTINUE
0029          READ(1,5)(A(I),B(I),C(I),D(I),I=1,3)
0030        5 FORMAT(4F15.7)
0031          PRINT 120
0032          PRINT 5,(A(I),B(I),C(I),D(I),I=1,3)
0033          PRINT 105
0034          DO 25 I=1,NAT
0035          IF(NTYP.EQ.1)GO TO 23
0036          READ(1,6)X(I),Y(I),Z(I),NAME(I)
0037          GO TO 24
```

```
A002 012620
$CO
0038        23 READ(1,7)NAME(I),X(I),Y(I),Z(I)
0039        24 PRINT 127,NAME(I),X(I),Y(I),Z(I)
0040        25 CONTINUE
0041           PRINT 128
0042        30 READ(1,8,END=99)NA,NB,NC,NE
0043           IF(NE)700,99,731
0044       731 PRINT 106,NA,NB,NC,NE
0045           TA=NA
0046           TB=NB
0047           TC=NC
0048           PRINT 111
0049           DO 40 I=1,NAT
0050           XC=TR(NE,1)+TA
0051           YC=TR(NE,2)+TB
0052           ZC=TR(NE,3)+TC
0053           XC=XC+S(NE,1,1)*X(I)+S(NE,1,2)*Y(I)+S(NE,1,3)*Z(I)
0054           YC=YC+S(NE,2,1)*X(I)+S(NE,2,2)*Y(I)+S(NE,2,3)*Z(I)
```



```
0055           ZC=ZC+S(NE,3,1)*X(I)+S(NE,3,2)*Y(I)+S(NE,3,3)*Z(I)
0056           XP=A(1)*XC+B(1)*YC+C(1)*ZC+D(1)
0057           YP=A(2)*XC+B(2)*YC+C(2)*ZC+D(2)
0058           ZP=A(3)*XC+B(3)*YC+C(3)*ZC+D(3)
0059           PRINT 110,NAME(I),XP,YP,ZP
0060        40 CONTINUE
0061       110 FORMAT(5X,A4,5X,3F10.4)
0062           GO TO 30
0063        99 STOP
0064         6 FORMAT(3F10.5,40X,A4)
0065         7 FORMAT(7X,A4,2X,3F8.4)
0066         8 FORMAT(4I3)
0067       120 FORMAT(34H0COORDINATE TRANSFORMATION MATRIX  /10X,2HVX,
```

A002 012620
$CO

```
            113X,2HVY,13X,2HVZ,13X,1HD  )
0068       105 FORMAT(/25H0INPUT ATOMIC COORDINATES  /
            138H0  ATOM          X          Y          Z     )
0069       127 FORMAT(2X,A4,2X,F12.4,2F10.4)
0070       128 FORMAT(1H0 )
```

```
0071        106 FORMAT(34H0CARTESIAN COORDINATES OF MOLECULE  /
              122H AFTER TRANSFORMATION./
              228H0EQUIVALENT POSITION CODE IS,1H(,4I4,1H))
0072        111 FORMAT(45H0      ATOM              X          Y          Z )
0073            END

        ROUTINES CALLED:
        EQPOS

        BLOCK        LENGTH
        MAIN.    2871    (013156)*
        .$$$$.   28      (000070)

        **COMPILER ----- CORE**
           PHASE        USED  FREE
        DECLARATIVES  00610 04535
        EXECUTABLES   00767 04378
        ASSEMBLY      01727 06335

#EQPA,KB:<CR:

FORTRAN V004A                          16:16:11    09-NOV-73   PAGE    1

0001            SUBROUTINE EQPOS(IEQ,RN,S)
0002            DIMENSION IEQ(45),NEQ(14),RN(3),S(3,3),R(3,2)
0003            COMMON NEQ
0004          2 FORMAT(//// @ IEQ(@,I2,@)=@,A1,@.  THIS IS NOT A LEGAL CHA
               1/@   THE ONLY ALLOWED CHARACTERS ARE @ 17(2X,A1))
0005            N=1
0006            K=1
0007            SS=1.
0008            DO 1 I=1,3
0009            R(I,1)=0.
0010            R(I,2)=1.
0011            DO 1 J=1,3
0012            S(I,J)=0.0
0013          1 CONTINUE
0014              DO 13 I=1,45
0015            DO 5 J=1,14
0016            IF(IEQ(I).EQ.NEQ(J)) GO TO 6

A002 012620
$CO
0017          5 CONTINUE
```

```
0018          PRINT 2,I,ILQ(I),(NEQ(J),J=1,15)
0019          STOP
0020        6 GO TO(7,7,7,8,9,10,11,12,12,12,12,12,13,14),J
0021        7 S(N,J)=SS
0022          GO TO 13
0023        8 N=N+1
0024          K=1
0025        9 SS=1.
0026          GO TO 13
0027       10 SS=-1.
0028          GO TO 13
0029       11 K=K+1
0030          GO TO 13
0031       12 R(N,K)=J-7
0032       13 CONTINUE

A002 012620
$CO

A002 012620
$CO
0033       14 DO 15 I=1,3
0034          RN(I)=R(I,1)/R(I,2)
0035       15 CONTINUE
0036          RETURN
0037          END

        BLOCK        LENGTH
        EQPOS   423     (001516)*
        .$$$$.  28      (000070)

        **COMPILER ----- CORE**
           PHASE        USED  FREE
        DECLARATIVES 00449 04696
        EXECUTABLES  00607 04538
        ASSEMBLY     01315 06747

#↑C
.I\I\KI
$RU LINK
LINK V11A01
#CARTES<CARTA,EQPA,FTNLIB/L/U/E

TRANSFER ADDRESS: 043750
```

```
LOW LIMIT: 043750
HIGH LIMIT: 077460

LINK V11A01
#↑C
.KI
$AS KB:,5
$AS CR,1
$RU CARTES


FORT001009 FILE DOES NOT EXIST / OR IS ALREADY OPEN
NAME     SEQ
MAIN.    00005

$AS KB:,5
$AS CR:,1
$RU CARTES

ANTHRACENE

    7 ATOMS INPUT.          4 EQUIVALENT POSITIONS.

INPUT EQUIVALENT POSITIONS.

 NO.
   1     X,Y,Z
   2     1/2&X,1/2-Y,Z
   3     -X,-Y,-Z
   4     1/2-X,1/2&Y,-Z

FORT006000 CONVERSION ERROR
NAME     SEQ
MAIN.    00029


COORDINATE TRANSFORMATION MATRIX
        VX            VY            VZ            D
    6.9016218    -2.6191590    -1.4314660    -0.0009930
   -2.7635620    -5.3858752    -0.8451320     0.0000000
   -4.2451401    -0.7520110    11.0385323    -0.0004630


INPUT ATOMIC COORDINATES
```

ATOM		Y	Z
A	0.0875	0.0291	0.3659
G	0.0041	0.1792	-0.3161
B	0.1189	0.1555	0.2806
F	0.0606	0.2587	-0.1824
C	0.0590	0.0821	0.1382
E	0.0301	0.1309	-0.0898
D	0.0874	0.2085	0.0473

CARTESIAN COORDINATES OF MOLECULE
AFTER TRANSFORMATION.

EQUIVALENT POSITION CODE IS(0 0 0 1)

ATOM	X	Y	Z
A	0.0034	-0.7076	3.6445
G	0.0101	-0.7093	-3.6419
B	0.0105	-1.4030	2.4753
F	0.0009	-1.4064	-2.4653
C	-0.0065	-0.7222	1.2123
E	-0.0071	-0.7122	-1.2185
D	-0.0113	-1.4044	-0.0065

CARTESIAN COORDINATES OF MOLECULE
AFTER TRANSFORMATION.

EQUIVALENT POSITION CODE IS(0 0 1 2)

ATOM	X	Y	Z
A	0.8654	-5.3145	12.2282
G	1.6587	-3.6987	5.1676
B	1.5347	-4.6481	11.2491
F	2.0656	-3.5402	6.4637
C	1.1334	-4.7574	9.8758
E	1.3881	-4.2224	7.5183
D	1.7905	-4.0786	8.8470

I350 000000

$

```
#
#↑C
.KI
$FI
TIME:-23:15:54

DOS V08-02

$
 $LO 40,1

DOS V08-02

$DA 12-NOV-73
$TI 10:03:00
$LO 40,1
DATE:-12-NOV-73
TIME:-10:03:08
$AS CR:,1
$AS KB:,5
$RU CARTES

ANTHRACENE

    7 ATOMS INPUT.          4 EQUIVALENT POSITIONS.

INPUT EQUIVALENT POSITIONS.

 NO.
   1     X,Y,Z
   2     1/2+X,1/2-Y,Z
   3     -X,-Y,-Z
   4     1/2-X,1/2+Y,-Z

COORDINATE TRANSFORMATION MATRIX
          VX              VY              VZ              D
     6.9016218      -2.6191590      -1.4314660      -0.0009930
    -2.7635620      -5.3858752      -0.8451320       1.0093020
```

-4.2451401 -0.7520110 11.0385323 -0.0004630

INPUT ATOMIC COORDINATES

ATOM	X	Y	Z
A	0.0875	0.0291	0.3659
G	0.0041	0.1792	-0.3161
B	0.1189	0.1555	0.2806
F	0.0606	0.2587	-0.1824
C	0.0590	0.0821	0.1382
E	0.0301	0.1309	-0.0898
D	0.0874	0.2085	0.0473

CARTESIAN COORDINATES OF MOLECULE
AFTER TRANSFORMATION.

EQUIVALENT POSITION CODE IS(0 0 0 1)

ATOM	X	Y	Z
A	0.0034	0.3017	3.6445
G	0.0101	0.3000	-3.6419
B	0.0105	-0.3937	2.4753
F	0.0009	-0.3971	-2.4653
C	-0.0065	0.2871	1.2123
E	-0.0071	0.2971	-1.2185
D	-0.0113	-0.3951	-0.0065

CARTESIAN COORDINATES OF MOLECULE
AFTER TRANSFORMATION.

EQUIVALENT POSITION CODE IS(0 0 1 2)

ATOM	X	Y	Z
A	0.8654	-4.3051	12.2282
G	1.6587	-2.6894	5.1676
B	1.5347	-3.6388	11.2491
F	2.0656	-2.5309	6.4637
C	1.1334	-3.7481	9.8758
E	1.3881	-3.2131	7.5183
D	1.7905	-3.0693	8.8470

I350 000000

$FI
TIME:-10:07:47

PROGRAM NAME CONTUR

PURPOSE contour Fourier

LIMITATIONS

SWITCH SETTINGS

LOGICAL UNITS default values

4 LP for headings on plot

5 DKO:CONTUR.DAT output from FOURR

6 KB for error output

7 input control card file

PF plot file

FILE ASSIGNMENTS

only if different from default

CONTUR

Program to contour electron density maps and Patterson Functions to the Versatec Matrix Printer/Plotter. The map input is generated as an option of program FOURR. In addition, the user must supply certain control information:

Input Check List:

1. GRID, NUMCOP, TITLE
2. NUMSKP, SYMTYP, XLEN, YLEN, BETA
3. SKIP CARDS
4. LEVEL CARDS
5. EOF CARD

```
C       USAGE:
C       ------
C               THIS PROGRAM USES FIVE DATASETS.  EACH DATA SET
C       HAS A DEFAULT VALUE WHICH MAY BE OVERRIDDEN AT RUN TIME.
C
C       LU      DEFAULT         USE
C       ------- --------------- ------------------------------
C       4       LP:             USED TO WRITE HEADINGS AFTER A
C                               PLOT.  IF HEADINGS NOT DESIRED
C                               IT MAY BE CHANGED TO THE TTY.
C       5       DK0:CONTUR.DAT  BINARY DATA FILE OF THE TYPE
C                               THAT FOURR PRODUCES.  ANY FILE
C                               THAT HAS THE RIGHT FORMAT MAY BE
C                               USED.  THE USER IS WARNED THAT
C                               THIS FILE NAME WILL BE OVERWRITTEN
C                               BY THE FOURR PROGRAM.  IF THE USER
C                               WISHES TO SAVE THE FOURR RESULTS,
C                               HE MAY RE-NAME THIS FILE,
C                               AND ASSIGN THE NEW FILE NAME TO UNIT
C                               FIVE FOR CONTOURING
C       6       KB:             USED FOR ERROR OUTPUT.
C       7       CR:             CONTROL FILE FOR CONTOURING.
C       PF      DK0:TEMCON      THIS IS THE PLOT FILE.  THE USER
C                               MAY RE-ASSIGN IT TO ANY PLOT FILE.
C                               A PLOT FILE MUST BE A CONTIGUOUS
C                               FILE ON AN RK DISC OF AT LEAST 256
C                               BLOCKS.
C
C       THE BINARY FILE HAS THE FOLLOWING FORMAT:
C       THE FIRST RECORD HAS 12 WORDS, AND SPECIFIES
C       THE SIZE OF THE GRID TO BE INPUT.
C       THE TWELVE WORDS ARE THREE SETS OF FOUR WORDS.  THE FIRST
C       DEALS WITH THE SECTION(PAGE TO PAGE), AND THE SECOND DEALS
C       WITH THE VERTICAL AXIS(DOWN THE PAGE), AND THE THIRD
C       DEALS WITH THE HORIZONTAL AXIS.  THE FOUR WORDS ARE INTEGERS
C       WITH THE FOLLOWING MEANING:
C       WORD 1: GRID SIZE
C       WORD 2: START POINT
C       WORD 3: NUMBER OF POINTS
C       WORD 4: INCREMENT
C
C       EACH BINARY RECORD FOLLOWING THAT HAS ALL THE DENSITY
C       VALUE FOR AN ENTIRE LINE.
C
C       THE CONTROL FILE CONTAINS THE FOLLOWING:
C
C                       - CONTROL CARD #1 -
C                       - CONTROL CARD #2 -
C                       - SKIP CARDS(IF ANY) -
C                       - LEVELS CARDS -
C                       - END OF FILE -
C       CONTROL CARD #1:
C       COL. 1:         'Y' OR 'N'.  'Y' SPECIFIES THE PRINTING
C                       OF AN ORTHOGONAL GRID ON THE CONTOUR.
C       COL. 2:         BLANK
C       COLS. 3-4:      NUMBER OF COPIES DESIRED OF EACH SECTION.
C       COLS. 5-16:     RESERVED.
C       COLS. 17-80:    TITLE FOR CONTOURS.
C       CONTROL CARD #2:
C       COLS. 1-3:      NUMBER OF SECTIONS TO SKIP(MAX=100).
C       COL. 4:         SYMMETRY TYPE:
C                       0=PLOT DATA AS GIVEN.
C                       1=TOP HALF OF DATA IS GIVEN, REFLECT ABOUT
C                         HORIZONTAL AXIS.
C                       2=BOTTOM HALF OF DATA IS GIVEN.
C                       3=LEFT HALF OF DATA IS GIVEN.
C                       4=RIGHT HALF OF DATA IS GIVEN.
C                       5=UPPER LEFT QUADRANT IS GIVEN.
C                       6=UPPER RIGHT QUADRANT IS GIVEN.
C                       7=LOWER LEFT QUADRANT IS GIVEN.
C                       8=LOWER RIGHT QUADRANT IS GIVEN.
C
C       COLS. 5-14:     X LENGTH
C       COLS. 15-24:    Y LENGTH:  Y-LEN/X-LEN IS THE RATIO
C                       OF THE AXIS.
C       COLS. 25-34:    ANGLE BETWEEN X AND Y(0 DEG<100).
C       SKIP CARDS(IF COLS 1-3 OF CARD 2 NON-ZERO).  ONE FOR
C       EACH SECTION TO BE SKIPPED.
C       COLS 1-6:       NUMBER OF THE SECTION TO BE SKIPPED.
C               SKIP CARDS MAY COME IN ANY ORDER.
C       LEVELS CARDS:
C       ONE FOR EACH LEVEL TO BE CONTOURED
C       COLS 1-6:       LEVEL TO CONTOUR.
```

CONTUR

Description of Input:

1. GRID, NUMCOP, TITLE (A1, 1X, I2, 12X, 64A1)

   GRID: 'Y' or 'N'. 'Y' requests the printing of an orthogonal grid over the contour.

   NUMCOP: Number of copies.

   TITLE: 64 character title.

2. NUMSKP, SYMTYP, XLEN, YLEN, BETA (I3, I1, 3F10.6)

   NUMSKP: number of skip cards

   SYMTYP:

Symtyp	Data supplied
0	All (for electron density use SYMTYP=0 only)
1	Left half
2	Right half
3	Top half
4	Bottom half
5	Upper left quadrant
6	Upper right quadrant
7	Lower left quadrant
8	Lower right quadrant

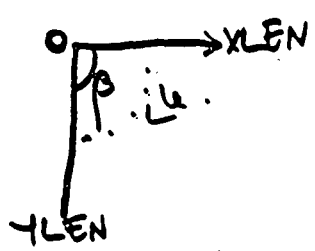
   * XLEN: Length of X-axis ~~divided by the length implied by the FOURR output~~. Across the page

   YLEN: Length of Y-axis ~~divided by the length implied by the FOURR output~~. Down the page

   BETA: Angle between X-axis and Y-axis. If $\beta \neq 0.0$ then SYMTYP is set to 0.

3. In any order, the skip cards (if any) specify any sections the user does not wish contoured. The format is I6.

4. Electron density contour interval cards specify the levels to be contoured. They must be in order, from lowest to highest. The format is I6.



Axis length down the page.

axis ~~cell~~ length horizontal

* CONTUR has to be set from starting values x = 0; y = 0; z = 0. It is not arbitrary (Ex the CONTUR can not be chosen from x: 0.5 y: 0.5 etc).

Contur grid pt limit is ≤ 61 × 61 pts across & down: Ex 44 × 84 is wrong

CONTUR

5. End of file. This is generated automatically on disc and magnetic tape files. On cards, this is a multipunch in column one (12-11-0-1-6-7-8-9) followed by a blank card. On the teletype this is done by typing a control 'D'.

More sophisticated users should refer to the program listing.

Sample input to CONTUR:

```
S*RU CONTUR
A005 007777
SAS KB:,7
SCO
*N  1          CTA FOURIER PHASED ON 15 ATOMS  R=26.6
*0070  91\1\.12      13.96      90.0
*4,
*5,
*6,
*7,
*8,
*9,
*10,
*10,
*20,
*30,
*40,
*50,
*60,
*70,
*80,
*90,
*↑D
```

CONTUR

Plot headings:

NS11 SHARPENED ORIGIN REMOVED PATTERSON
SECTION 13

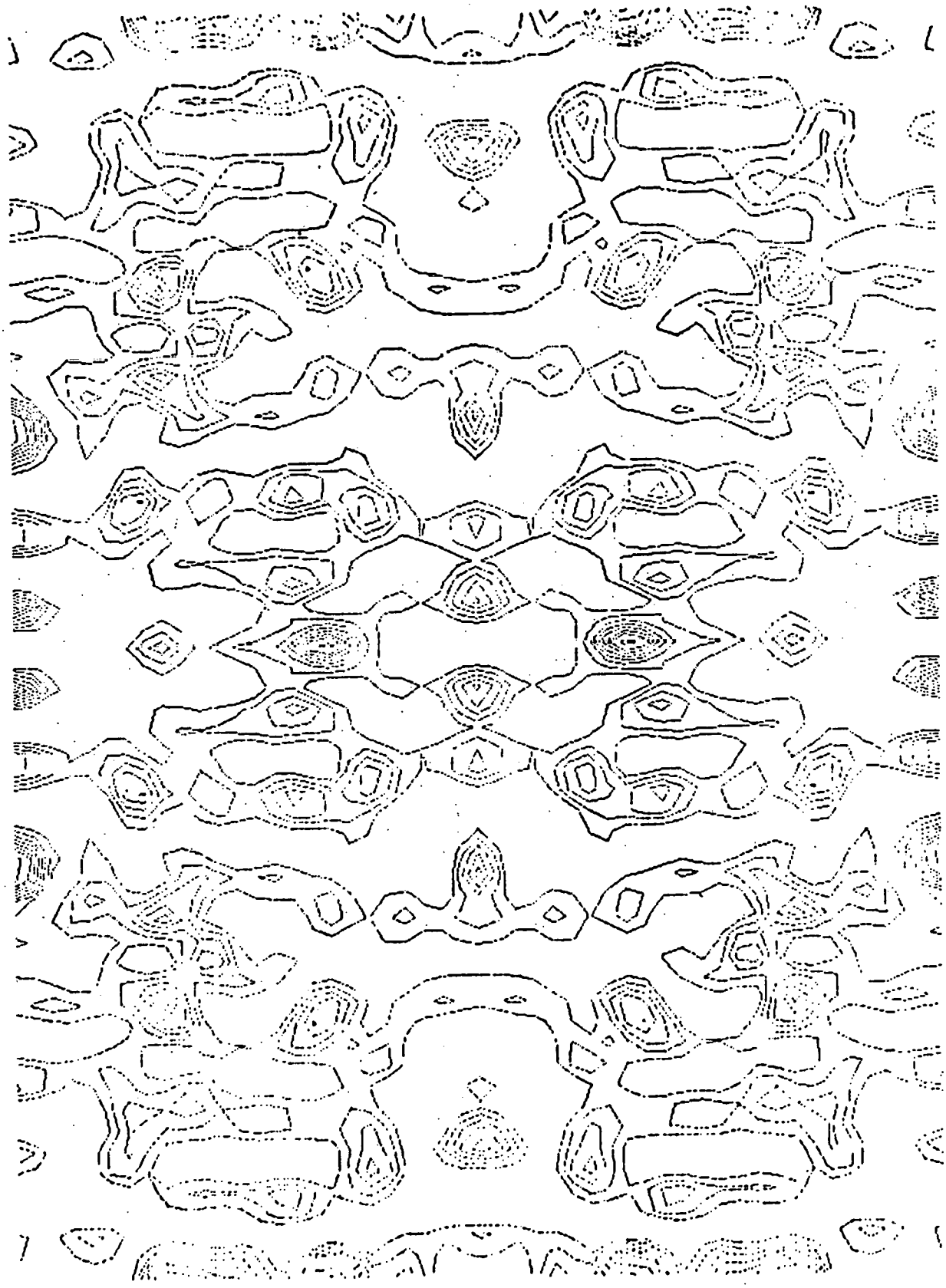
	GRID	START	# OF PTS.	INCREMENT
SECTION	24	0	13	1
VERTICAL	50	0	26	1
HORIZONTAL	60	0	31	1

SYMMETRY TYPE: 5
X-LENGTH : 1.00000000
Y-LENGTH : 0.72489089
BETA : 90.000000

10 LEVELS.
0 50 100 150 200 250 300 400 600 800

CONTUR

Sample Plot Output:



COINC - coincidence correction

Card 1 # of points (I5)
Card 2 MAsitling 3intensities at Weak, medium, Strong
(F5.2, 3F10.0)

COMPC

```
C
      REAL IO,IT,IC
      DIMENSION IO(20,3),IT(20,3),IC(20,3),RAT(20),T(20)
      DIMENSION AMP(20)
    1 FORMAT(I5)
    2 FORMAT(F5.2,3F10.0)
    3 FORMAT(F9.2,3F15.1)
    4 FORMAT(61H0      MA              I(WEAK)          I(MED)      S
     1RONG)  )
    5 FORMAT( 5H0TAU=,F16.8  ,30H(FROM SETTINGS I(3) GE 10000.))
    6 FORMAT(41H0   MA        I(OBS)       I(T)         I(C)  )
    7 FORMAT(F6.2,3F12.0)
    8 FORMAT( 5H0TAU=,F16.8,39H0(FROM HIGHEST SETTING FOR STRONE
    9 FORMAT(5H0TAU=,F12.8,39H0(FROM ALL SETTINGS OF STRONG PEAK
      F=10000.
C 888 READ(5,1)NSET
  888 READ(1,1)NSET
      IF(NSET.LE.0)GO TO 501
      WRITE(6,4)
      DO 10 I=1,NSET
C     READ(5,2)AMP(I),IO(I,1),IO(I,2),IO(I,3)
      READ(1,2)AMP(I),IO(I,1),IO(I,2),IO(I,3)
      IO(I,1)=0.01*IO(I,1)
      IO(I,2)=0.1*IO(I,2)
      IO(I,3)=0.1*IO(I,3)
      WRITE(6,3)AMP(I),(IO(I,J),J=1,3)
      RAT(I)=IO(I,1)/IO(1,1)
   10 CONTINUE
      DO 11 I=1,NSET
   11 IT(I,2)= IO(1,2)*RAT(I)
      DO 12 I=2,NSET
      IF(IO(1,3)-IO(I,2))13,13,12
   12 CONTINUE
   13 N=I-1
      FRAC=(IO(1,3)-IO(N,2))/(IO(I,2)-IO(N,2))
      FTT=IT(N,2)+FRAC*(IT(I,2)-IT(N,2))
      IT(1,3)=FTT
      DO 14 I=2,NSET
   14 IT(I,3)=FTT*RAT(I)
C
C     TAU FROM HIGHEST SETTING OF STRONG PEAK.
C
      TAU=(IT(NSET,3)-IO(NSET,3))/(IT(NSET,3)**2)
      WRITE(6,8)TAU
      NT=1
      GO TO 40
C
C     TAU CALCULATED FROM ALL SETTINGS FOR STRONG PEAK.
C
```

```
0040        25 NT=2
0041           STAU=0.0
0042           DO 15 I=1,NSET
0043           ANUM=IT(I,3)-IO(I,3)
0044           DEN=IT(I,3)**2
0045           T(I)=ANUM/DEN
```



```
0046        15 STAU=STAU+T(I)
0047           FN=NSET
0048           TAU=STAU/FN
0049           WRITE(6,9)TAU
0050           GO TO 40
        C
        C      TAU CALCULATED FROM SETTINGS WHERE INTENSITY GT. OR EQ. 10
        C
0051        26 NT=3
0052           STAU=0.0
0053           FN=0.
0054           DO 30 I=1,NSET
0055           DO 29 J=2,3
0056           IF(IO(I,J)-F)29,28,28
0057        28 STAU=STAU+(IT(I,J)-IO(I,J))/(IT(I,J)**2)
0058           FN=FN+1.
0059        29 CONTINUE
0060        30 CONTINUE
0061           TAU=STAU/FN
0062           WRITE(6,5)TAU
0063        40 WRITE(6,6)
0064           DO 16 I=1,NSET
0065           DO 17 J=1,3
0066        17 IC(I,J)=(1.0-SQRT(1.0-4.0*TAU*IO(I,J)))/(2.0*TAU)
0067        16 CONTINUE
0068           DO 20 I=1,NSET
0069           WRITE(6,7)AMP(I),IO(I,2),IT(I,2),IC(I,2)
0070           WRITE(6,7)AMP(I),IO(I,3),IT(I,3),IC(I,3)
0071        20 CONTINUE
0072           GO TO (25,26,50),NT
0073        50 GO TO 888
0074       501 CALL EXIT
0075           END

        ROUTINES CALLED:
        SQRT  , EXIT

        BLOCK        LENGTH
        MAIN.    1563    (006066)*

        **CO[illegible] CORE**
```

```
COMPILER
        PHASE          USED   FREE
DECLARATIVES  00446  04705
EXECUTABLES   00687  04464
ASSEMBLY      01600  06468

#↑C
.KIL
$RUN PIP
PIP-11   V7A01
#/DI

DIRECTORY DK0: [ 40,1   ]

02-NOV-73

HELEN .MES      1   01-NOV-73 <233>
FORTRN.LDA     29   02-NOV-73 <233>
EDIT  .LDA     13   02-NOV-73 <233>
LINK  .LDA     14   02-NOV-73 <233>
BUD             1   02-NOV-73 <233>
GRAPH .FTN      1   02-NOV-73 <233>
FTNLIB.OBJ    120   02-NOV-73 <233>
GRAPH .OBJ      2   02-NOV-73 <233>
QUAD  .FTN      1   02-NOV-73 <233>
QUAD  .OBJ      1   02-NOV-73 <233>
COINC .OBJ     16   02-NOV-73 <233>
RUNPIP          1   02-NOV-73 <233>

TOTL BLKS:    200
TOTL FILES:    12


#↑C
.KIL
$RUN LINK
LINK V11A01
#COINC<COINC,FTNLIB/L/E

TRANSFER ADDRESS: 052454
LOW LIMIT: 052454
HIGH LIMIT: 077460

LINK V11A01
#↑C
.KI
$AS CR:,1
$RUN COINC
```

MA	I(WEAK)	I(MED)	I(STRONG)
4.50	844.4		502.0

6.00	1169.2	6788.4	16136.3
7.80	1486.0	8640.3	20655.4
9.50	1827.5	10515.1	25022.2
12.80	2518.4	14121.4	33420.8
15.30	3019.1	16806.5	39524.7
19.50	3791.6	21275.2	49463.3
22.30	4278.3	23924.6	55070.4
25.50	4965.9	27443.2	62557.4

TAU= 0.000001550(FROM HIGHEST SETTING FOR STRONG PEAK)

MA	I(OBS)	I(T)	I(C)
4.50	4864.	4864.	4901.
4.50	11792.	11936.	12016.
6.00	6788.	6735.	6861.
6.00	16136.	16527.	16561.
7.80	8640.	8560.	8759.
7.80	20655.	21005.	21363.
9.50	10515.	10527.	10692.
9.50	25022.	25833.	26076.
12.80	14121.	14507.	14445.
12.80	33421.	35598.	35358.
15.30	16806.	17391.	17269.
15.30	39525.	42676.	42297.
19.50	21275.	21840.	22027.
19.50	49463.	53594.	53979.
22.30	23925.	24644.	24884.
22.30	55070.	60474.	60799.
25.50	27443.	28605.	28722.
25.50	62557.	70194.	70194.

TAU= 0.000001370(FROM ALL SETTINGS OF STRONG PEAK)

MA	I(OBS)	I(T)	I(C)
4.50	4864.	4864.	4897.
4.50	11792.	11936.	11989.
6.00	6788.	6735.	6853.
6.00	16136.	16527.	16511.
7.80	8640.	8560.	8745.
7.80	20655.	21005.	21277.
9.50	10515.	10527.	10672.
9.50	25022.	25833.	25947.
12.80	14121.	14507.	14407.
12.80	33421.	35598.	35115.
15.30	16806.	17391.	17214.
15.30	39525.	42676.	41941.
19.50	21275.	21840.	21936.
19.50	49463.	53594.	53378.
22.30	23925.	24644.	24767.
22.30	55070.	60474.	60019.
25.50	27443.	28605.	[illegible]

25.50	62557.	70194.	285647
			69121.

TAU= 0.00000134(FROM SETTINGS I(3) GE 10000.)

MA	I(OBS)	I(T)	I(C)
4.50	4864.	4864.	4896.
4.50	11792.	11936.	11984.
6.00	6788.	6735.	6851.
6.00	16136.	16527.	16500.
7.80	8640.	8560.	8742.
7.80	20655.	21005.	21259.
9.50	10515.	10527.	10667.
9.50	25022.	25833.	25919.
12.80	14121.	14507.	14398.
12.80	33421.	35598.	35062.
15.30	16806.	17391.	17202.
15.30	39525.	42676.	41865.
19.50	21275.	21840.	21916.
19.50	49463.	53594.	53249.
22.30	23925.	24644.	24742.
22.30	55070.	60474.	59853.
25.50	27443.	28605.	28530.
25.50	62557.	70194.	68894.

$

PROGRAM NAME	DECAY
PURPOSE	calculated the decay curve for data and plots the curve on the VERSATEC printer/plotter
LIMITATIONS	
SWITCH SETTINGS	
LOGICAL UNITS	6--KB for input information
FILE ASSIGNMENTS	none necessary log in as [1,11]

DECAY

A program to calculate first and second order decay curves from the observed intensities of check reflections. The program will also produce plots of the standard intensities as a function of time. The reflections used are those read onto file STDFIL [1,11] by the program RSTD. In order to run tiis program with plotting, it is necessary for the user to log in under [1,11]. The only input supplied by the user at execution time is via the teletype and is described below.

INPUT: (via TTY)

TITLE (40H)

run identification

NSTD, NTOT, ISTRT (3I5)

NSTD - No. of check reflections (≤10)

NTOT - Total No. of check reflections on the STDFIL [1,11]. (this no. is supplied by program RSTD.)

If the user desires to use some no. of data less than the no. of data on the file then NTDT may be less than on the file, however, the following must be true:

NTØT(MODULO (NSTD)) = 0.

ISTRT - Number of the first check reflection which is to be used in the calculation for the current run. This has been done so that if a user wishes to use only a portion of the data, he may specify the check reflections to be included. All reflections included in the range ISTRT to NTDT will be used.

* H,K,L SINTEN (3I5, F10.2)

The h,k,ℓ and initial intensity of the deck reflection, there must be 1 entry for each of the NSTD check reflections.

one line for each refl^n; it can be had from RSTD list

1 h, k, l, xxxx. . .

2 . . .

3 . . .

4 . . .

DECAY

The remaining input concerns the plotting of the check reflection information. When the analysis of the check reflections is complete, the following will be printed on the teletype:

PLOT DECAY CURVES (BLANK-YES)*

if plots are to be made then carriage return
if plots are not wanted, type in NO <Cr>
if curves are to be plotted, the following will be printed on the TTY:

ENTER PLOTFILE FILENAME..*
Type in TEMCON <Cr>

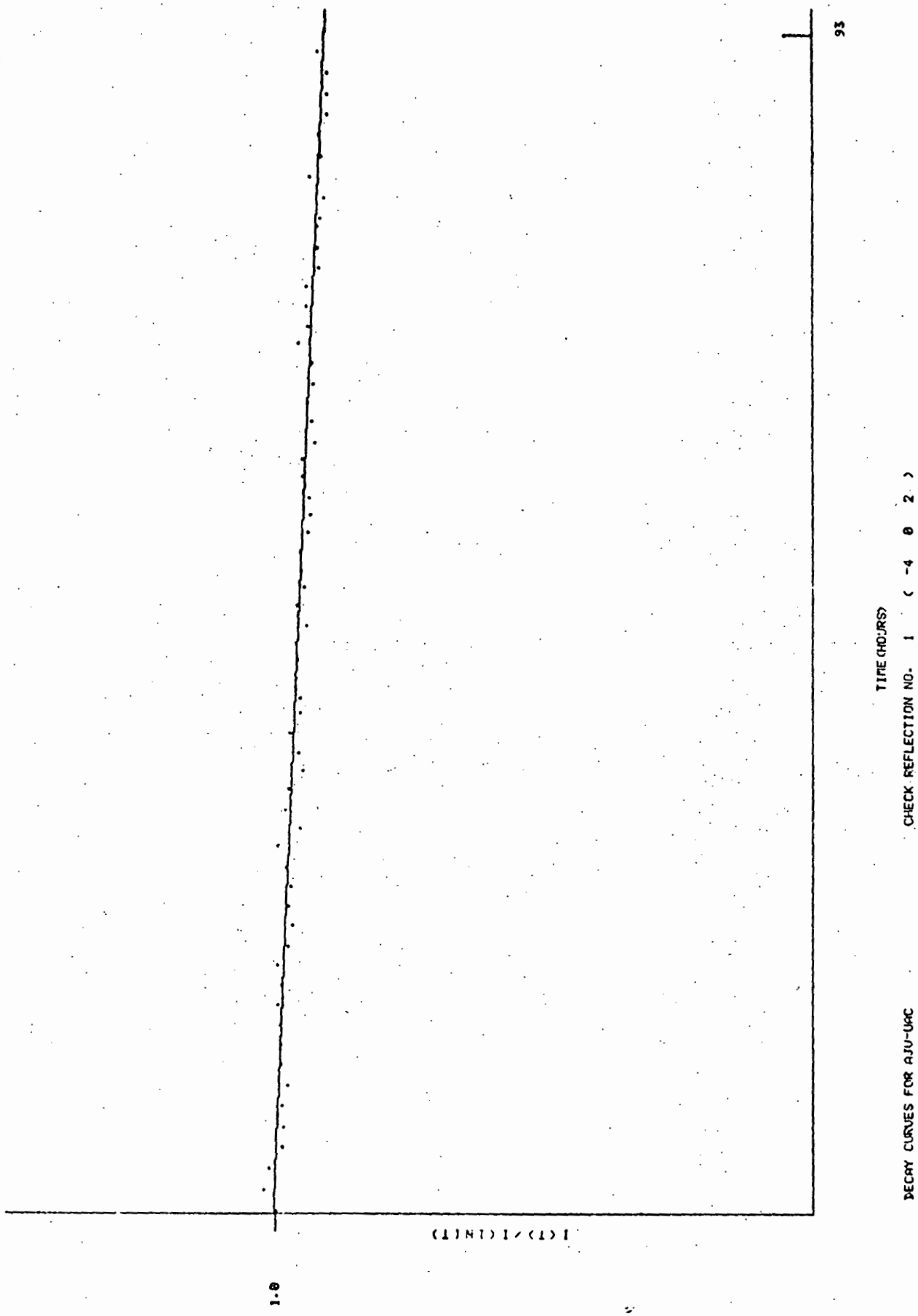
DECAY

Sample input
(N.B. must log in as 1, 11; no file assignments are required)

```
RUN DECAY

ENTER RUN IDENTIFICATION(UP TO 40 CHARACTERS)
*DECAY TEST  LAMBDAS DATA

INPUT NSTL,NTOT,ISTRT..*4,52,1,

ENTER H,K,L, AND INITIAL INTENSITIES FOR
 4 CHECK REFLECTIONS.
*0,0,2,386144.
*0,6,0,103359.
*2,0,0,3402338.
*3,3,0,3282671\7\3.

PLOT DECAY CURVES(BLANK=YES) *

ENTER PLOTFILE FILENAME..*TEICON

(*
```

DECAY

Sample Plot



PROGRAM NAME	EXTCAL
PURPOSE	calculate extinction correction
LIMITATIONS	
SWITCH SETTINGS	
LOGICAL UNITS	7 HKL data usually DKØ or MTØ 1 input control information
FILE ASSIGNMENTS	1 and 7 must be assigned

```
      EXTCAL...
      PROGRAM TO CALCULATE SECONDARY EXTINCTION COEFFICIENT
      USING THE FILE OF OBSERVED AND CALCULATED STRUCTURE FACTORS
      WRITTEN BY THE STRUCTURE FACTOR CALCULATION PROGRAM.

      DIMENSION TITLE(18)
      NRIT=1
      NWOT=5
      NHKL=7
      CALL SETFIL(NRIT,'D',IOERR,'CR')
      CALL SETFIL(NWOT,'D',IOERR,'LP')
      CALL SETFIL(NHKL,'HKLDAT.DAT',IOERR,'DK',0,0)
      READ(NRIT,1)TITLE
      FORMAT(18A4)
      READ(NRIT,2)S1,S2,S3,S4,S5,S6
      READ(NRIT,2)TTM,ALAM,FOMIN,SCALE
      FORMAT(6F10.6)
      S1,S2,S3,S4,S5,S6... THESE ARE THE COEFFICIENTS FOR THE
      CALCULATION OF SIN(THETA)**2/LAMBDA**2 BY THE
      EQUATION SSO=S1*H*H+S2*K*K+S3*L*L+S4*H*K+S5*H*L+S6*K*L
      TTM...2-THETA OF THE MONOCHROMATOR
      ALAM...X-RAY WAVELENGTH(ANGSTROMS)
      FOMIN... MINIMUM VALUE OF FOBS TO BE USED IN THE CALCULATION
      SCALE... SCALE FACTOR TO PLACE FOBS ON ABSOLUTE SCALE

      ALAM2=ALAM*ALAM
      COSM=COS(PI*TTM/180.)
      CTM=COSM*COSM
      NUSE=0
      NDAT=0
      SUMALP=0.
      SUMW=0.
      SUMWAL=0.
      WRITE(NWOT,10)TITLE
   10 FORMAT(/' SECONDARY EXTINCTION COEFFICIENT DETERMINATION'//
     11X,18A4)
      WRITE(NWOT,11)S1,S2,S3,S4,S5,S6
   11 FORMAT(//' THE INPUT COEFFICIENTS FOR THE CALCULATION
     1 OF SIN(THETA)**2/LAMBDA**2 ARE;'/' S1='F10.6,'    S2='
     2F10.6'    S3='F10.6'    S4='F10.6'    S5='F10.6'    S6='
     3F10.6/)
      WRITE(NWOT,12)TTM,ALAM,FOMIN,SCALE
   12 FORMAT(' 2-THETA OF MONOCHROMATOR ='F8.2/' X-RAY WAVELENGTH='
     1F9.5/' FOB(MINIMUM)='F10.3/' SCALE FACTOR ='F10.5)
      WRITE(NWOT,13)
   13 FORMAT(///'   H    K    L     SINL       FOB      FCAL     FC/FO
     1        IOBS       BETA      BETA*IOBS          ALPHA')
   20 READ(NHKL,END=30)IH,IK,IL,NOT,FOB,FCAL,DLF,PHI
      NDAT=NDAT+1
      IF(FOB-FOMIN)20,21,21
   21 FJ=IH
      FK=IK
      FL=IL
      FOS=(FOB/SCALE)**2
      SSO=FJ*FJ*S1+FK*FK*S2+FL*FL*S3+FJ*FK*S4+FJ*FL*S5+FL*FK*S6
      SINL=SQRT(SSO)
      SSO=SSO*ALAM2
      COSO=1.0-SSO
      CST=1.0-4.0*SSO*COSO
      STT=2.0*SQRT(SSO*COSO)
      BETA=(1.0+CTM)*(1.0+CTM*CST+CST)/((1.0+CTM*CST)**2)
      P1=(CTM+COSO)/(1.0+CTM)
      P2=(COSM+COSO)/(1.0+COSM)
```

These are coefficients from DATRDN-XRAY-72

```
      FLP=0.5*(P1+P2)/STT
      SJOBS=FOS+FLP
      FRAT=FCAL/FOB
      BETAJ=BETA*SJOBS
      ALPHA=(FRAT-1.0)/BETAJ
      WRITE(NWOT,4)IH,IK,IL,SINL,FOB,FCAL,FRAT,SJOBS,BETA,BETAJ,
     1ALPHA
      SUMALP=SUMALP+ALPHA
      SUMW=SUMW+BETAJ
      SUMWAL=SUMWAL+ALPHA*BETAJ
      NUSE=NUSE+1
      GOTO 20
      FORMAT(3I4,F8.4,2F9.2,F9.4,F12.0,F10.4,F12.0,E15.5)
   30 WRITE(NWOT,5)NDAT,NUSE
      FORMAT(/I5' DATA READ FROM REFLECTION FILE.     'I5' DATA
     1 WITH FOB.GE.FOMIN.')
      ALP1=SUMALP/(FLOAT(NUSE))
      ALP2=SUMWAL/SUMW
      WRITE(NWOT,6)ALP1,ALP2
      FORMAT(//' AVERAGE VALUE FOR ALPHA(UNWEIGHTED) ='E15.5/
     1' AVERAGE VALUE FOR ALPHA(WEIGHTED) ='E15.5)
      REWIND NHKL
      END
```

Sample Input:

```
F032 100000
$↑C
.KI
$*AS DK0:HKL.DAT,\,\.DAT,7    ←File with HKL Data
$*AS KB:,1
$*RU EXR\R\TCAL[40,1]
*
*.003004,.001282,.003328,
*26.3,1.5418,30.,.14066

$*
```

PROGRAM NAME	ELLIPS
PURPOSE	displays molecules with thermal ellipsoids
LIMITATIONS	50 atoms anisotropic 160 atoms isotopic
SWITCH SETTINGS	
LOGICAL UNITS	1 input atomic parameter 6 KB
FILE ASSIGNMENTS	1 must be assigned to CR, DKØ or MTØ

ELLIPS

PROGRAM - ELLIPS] All input on unit 1-- must be assigned additional entries on KB

Program to compute atomic vibration parameters from temperature factors and to display the results on the Vector General display. An input file is required consisting of 1) a title card, 2) cell parameters and 3) the coordinates and temperature factors. Some other input is required through the teletype. The limits are 50 atoms anisotropic or 160 atoms isotropic. The following relation must also hold.

NAN = number anisotropic atoms
NISO = number isotropic

$$16\ (NAN) + 5\ (NISO) \leq 800$$

The input file is expected on logical unit #1 and must have the following organization:

1. RUN TITLE (up to 60 characters - 15A4)
2. a, b, c, α, β, γ (direct cell parameters 6F10.5)
3. coordinates and temperature factors
   (a) coordinate card
   X, Y. Z, LABEL
   fractional coordinates and atom label
   (b) β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}, ITYPE

ITYPE = 0 } as for anisotropic thermal parameters in
ITYPE = 1 } ORTEP

ELLIPS

E = 6 as for isotropic thermal parameters

ITYPE = 7 in ORTEP

for the coordinate cards, the label may be either first or last and the format is specified at run time through the teletype.

The format of the temperature factor cards is specified at run time. However, remember that even for isotropic temperature factors, 6 β_{ij}'s will be read even though only β_{11} is to be used as the isotropic temperature factor.

Various options concerning the display of the atom array and printing of output are available at run time and are self explanatory at execution time.

The dials on the display have the following functions.

1, 2 and 3	rotation about X, Y, and Z
, 5	control intensity and window
6, 7	scale
8, 9, 10	translation of X, Y, and Z

The following is a sample run of the program.

ELLIPS

Sample input for logical unit 1

```
 MCLMSZ  MO  ULES A AND B
20.449.11.47  3.035.90..108.91.90..
  -.19492   .00049   .21640            1.00000 1                    C 1B
   .00239   .01484   .00909  -.00139   -.00052   .00530  1         C 1B
   .09764   .11078   .33855            1.00000 2                    C 1B
   .00197   .00934   .00464   .00152    .00138   .00169  1         C 1B
   .10515   .00160   .29270            1.00000 2                    C 2B
   .00247   .01032   .00491   .00260    .00172  -.00093  1         C 2B
   .05384  -.00540   .27862            1.00000 2                    C 3B
   .00337   .01017   .00557   .00193    .00116  -.00282  1         C 3B
  -.00561  -.05410   .30097            1.00000 2                    C 4B
   .00294   .00843   .00588   .00112    .00068  -.00193  1         C 4B
  -.14850   .19105   .45001            1.00000 2                    C 5B
   .00344   .01068   .00890   .00458    .00576   .00419  1         C 5B
  -.15227   .28355   .51077            1.00000 2                    C 6B
   .00498   .01236   .01035   .00518    .00747   .00605  1         C 6B
  -.03569   .35107   .55365            1.00000 2                    C 7B
   .00560   .00993   .01004   .00519    .00877   .00393  1         C 7B
  -.03377   .34143   .53476            1.00000 2                    C 8B
   .00533   .00798   .00732   .00339    .00645   .00169  1         C 8B
   .03537   .22153   .44357            1.00000 2                    C 9B
   .00334   .00649   .00476   .00032    .00127   .00101  1         C 9B
  -.07569   .06217   .37692            1.00000 2                    C10B
   .00307   .00777   .00524   .00000    .00167   .00106  1         C10B
   .03349   .12830   .37888            1.00000 2                    C11B
   .00195   .00562   .00439   .00088    .00108   .00137  1         C11B
  -.01555   .04353   .35172            1.00000 2                    C12B
   .00103   .00702   .00418   .00043    .00034  -.00043  1         C12B
  -.08374   .16512   .43034            1.00000 2                    C13B
   .00234   .00859   .00623   .00191    .00306   .00281  1         C13B
  -.02550   .24149   .47155            1.00000 2                    C14B
   .00301   .00674   .00578   .00094    .00315   .00046  1         C14B
   .09740   .29666   .50849            1.00000 2                    C15B
   .00324   .00825   .00703  -.00193    .00067  -.00158  1         C15B
  -.13375  -.02663   .34993            1.00000 2                    C16B
   .00215   .01139   .00592  -.00205   -.00022   .00274  1         C16B
   .14344   .20336   .33355            1.00000 2                    C17B
   .00165   .01326   .00622  -.00004    .00118   .00484  1         C17B
   .15650   .18163   .29325            1.00000 2                    C18B
   .00250   .01741   .00631   .00151    .00230   .00559  1         C18B
   .20793   .07072   .25617            1.00000 2                    C19B
   .00191   .01933   .00653   .00282    .00344   .00348  1         C19B
   .16198  -.01863   .25455            1.00000 2                    C20B
   .00301   .01600   .00663   .00468    .00265  -.00048  1         C20B
   .69945   .49551   .43159            1.00000 1                    C 1A
   .00245   .01416   .00930  -.00108    .00484  -.00045  1         C 1A
   .40347   .39182   .24510            1.00000 2                    C 1A
   .00321   .00805   .00601   .00028    .00323  -.00263  1         C 1A
   .39704   .50342   .19406            1.00000 2                    C 2A
   .00235   .01097   .00592   .00139    .00327  -.00192  1         C 2A
   .45074   .58936   .23151            1.00000 2                    C 3A
   .00288   .01067   .00608  -.00007    .00337  -.00006  1         C 3A
   .50952   .55150   .31361            1.00000 2                    C 4A
   .00271   .00838   .00709  -.00004    .00430   .00123  1         C 4A
   .64690   .29944   .60624            1.00000 2                    C 5A
   .00349   .00983   .00662   .00182    .00236   .00064  1         C 5A
   .65060   .20417   .66882            1.00000 2                    C 6A
   .00499   .01098   .00759   .00264    .00383   .00086  1         C 6A
   .59285   .13016   .65246            1.00000 2                    C 7A
   .00438   .01065   .00720   .00196    .00286   .00277  1         C 7A
   .53211   .15234   .57177            1.00000 2                    C 8A
   .00521   .00735   .00923  -.00088    .00723  -.00022  1         C 8A
   .46425   .27736   .41596            1.00000 2                    C 9A
```

ELLIPS

Sample input for logical unit 1, ctd.

.00242	.00539	.00692	-.00167	.00438	-.00272	1	C 9A
.57738	.3126	.45033		1.00000	2		C10A
.00208	.0791	.00588	-.00126	.00329	-.00202	1	C10A
.46119	.36668	.34427		1.00000	2		C11A
.00175	.00709	.00638	-.00079	.00351	-.00281	1	C11A
.51768	.45356	.37339		1.00000	2		C12A
.00215	.00722	.00551	-.00064	.00344	-.00052	1	C12A
.59276	.33532	.52058		1.00000	2		C13A
.00167	.00719	.00564	.00036	.00348	-.00025	1	C13A
.51550	.25313	.50125		1.00000	2		C14A
.00299	.00665	.00599	-.00019	.00481	-.00108	1	C14A
.40068	.20264	.41229		1.00000	2		C15A
.00294	.00796	.01088	-.00343	.00580	-.00284	1	C15A
.63410	.52167	.49550		1.00000	2		C16A
.00199	.00867	.00774	-.00264	.00359	-.00300	1	C16A
.35436	.30323	.19166		1.00000	2		C17A
.00180	.01197	.00826	-.00188	.00295	-.00729	1	C17A
.26569	.33031	.09754		1.00000	2		C18A
.00345	.01240	.00777	.00129	.00325	-.00502	1	C18A
.29003	.44139	.05391		1.00000	2		C19A
.00285	.01954	.00691	.00224	.00243	-.00654	1	C19A
.33504	.52925	.09902		1.00000	2		C20A
.00294	.01418	.00694	.00230	.00293	-.00221	1	C20A

PROGRAM NAME FOURR

PURPOSE calculates Fourier synthesis

LIMITATIONS

SWITCH SETTINGS

LOGICAL UNITS Defaults

1 - CR input file (see check list)
2 - DKO:CONTUR.DAT (if contouring as specified)
4 - DKO:TEMCON[1,11] temporary file for I/O
5 - LP
6 - KB

FILE ASSIGNMENTS

only if different from default

PROGRAM: FOURR New Version 5/1/75

PURPOSE: Calculation of Fourier synthesis

MACHINE: PDP 111/40 (DOS-VØ8) 28K

DESCRIPTION: FOURR is a program to be used for the computation of crystallographic Fourier syntheses. This version of the program is intended for use for triclinic, monoclinic or orthorhombic space groups. The program consists of the main routine and five (5) overlays. The overlay programs and their functions are:

OVERLAY	Function
SYMMET	Input of necessary Fourier control information
EXPAND	Expands reflection data to simulate space group P1
NCFOU	Fourier summation
FOUPRT	Prints Fourier and writes file for contouring program
PECKIT	Searches the Fourier for the electron density maxima greater than a user specified value

The communication between the overlays is accomplished by labeled common and temporary data files. The following files are used in the course of a run:

LU.	File:	Data Type
1	CR:	Fourier control information
5	LP:	Printed output
7	DKØ:FOURR:DAT	Reflection data file, normally written by CALCSF or PATT
3	MTØ:SCRACH,DAT	Floating point output of Fourier synthesis. This file has been relegated to a magnetic tape due to the usually limited available disk space
4	TEMCON[1,11]	This is the file to which the expanded reflection data are WRITTEN where they are used by the summation routine. TEMCON must be a file of at least 512 contiguous tracks of 256 words.
2	DKØ:CONTUR,DAT	Integer output file of the electron density map and is used by the contouring program CONTUR
1(8)	DKØ:PEAKER,DAT	Output file of electron density maxima providing the peak search overlay. PECKIT is used.

The user must supply the control information on punched cards, a disk file of reflection data, namely FOURR,DAT under the current [UIC] and a magnetic scratch tape on MTØ:. The remaining files are assigned by the program and if either CONTUR,DAT or PEAKER,DAT files are present on the disk under the [UIC], they will be deleted from the directory and replaced by the files generated by the current run.

LIMITATIONS:

6896 Expanded reflection data

61 Calculated grid points in either direction within the grid sections

500 Electron density maxima

CARD INPUT:

I. Title

II. Control card 1

III. Control card 2

IV. Symmetry cards

V. Grid card

VI. Peak search parameters

I. TITLE (15A4)

II. MAPANS,CONANS,NTYP,NEQ,MAXH,MAXK,MAXL,IORDX,IOFDY,IORDZ,NSPAC,NCOL,PRMAX
(2A1,10I4,F9.Ø)

MAPANS	= N	Do not print map
	= Y	Print map
CONANS	= 1	F_{OBS} MAP
	= 2	F_{CALC} MAP
	= 3	ΔF MAP
	= 4	F^2_{OBS} MAP
NEQ		Number of symmetry cards exclusive of lattice centering or center of symmetry. These are the unique summetry relations as given by the International Tables, Vol. I.
MAXH,MAXK,MAXL		The maximum values at /h/,/k/,/l/ respectively to be used in the map
IORDX	= 1	if x-axis to be page to page
	= 2	if x-axis to be vertical on the page (down the page)
	= 3	if x-axis to be across the page
IORDY,IORDZ		as for IORDX but referring to y- and z-axes

(IORDX+IORDY+IORDZ=6)

NSPAC	= 1	single space printed map
	= 2	double space printed map
NCOL	= 3	3 print columns/density point
	= 4	4 " " " "
PRMAX	≤Ø.Ø	do not rescale density map for printing or for CONTUR.DAT
	>Ø.Ø	scale the density for printout so that the point of maximum density printed is = PRMAX (normally Ø.Ø)

The default values for NSPAC is 1 and for NCOL the default is 3. Default PRMAX is Ø.Ø however if NCOL=3, all density points >999 are printed as 999 and if NCOL=4 if ρ>9999 ρ is set to 9999.

III. VOLUME,FOMAX,FLMAX,DFMAX (4F10.5)

IV. Symmetry Cards: (30A1)
NEQ CARDS

Punched as in International Tables as for CALCSF
e.g. space group $P2_1/C$
X,Y,Z
-X,1/2+Y,1/2-Z

V. NX,NSX,NNX,NDX,NY,NSY,NNY,NDY,NZ,NSZ,NNZ,NDZ,SCALE,FZRO,PRMIN

VI. NOPIK,RHOMIN (I1,F9.Ø)

NOPIK = 0 Do not search for electron density maxima
≠ 1 Search for electron density maxima

RHOMIN Minimum value of $\rho(xyz)$ to include in the search. Values of ρ<RHOMIN are ignored.

PROGRAM NAME HKLTRN

PURPOSE This program transforms the h, k, l indicies of a set of reflection data so that axes may be interchanged or lattice centering changed.

LIMITATIONS One transformation matrix; Two lattice conditions

SWITCH SETTINGS None

LOGICAL UNITS KB: is 1. The matrix (etc.) is input from the keyboard.

FILE ASSIGNMENTS Assign the input data (magnetic tape or disc file usually) to unit 7.

HKLTRN

Input: Assign a binary data tape or file with the name list IH, IK, IL, NOT, (F(I), I = 1,13) to file 7. (see example).

1. Transformation matrix 9F8.3

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ b_{21} & b_{22} & b_{23} \\ c_{31} & c_{32} & c_{33} \end{vmatrix} \begin{vmatrix} h \\ k \\ l \end{vmatrix}$$

$$h' = a_{11}h + a_{12}k + a_{13}l$$

$$k' = b_{21}h + b_{22}k + b_{23}l$$

$$l' = c_{31}h + c_{32}k + c_{33}l$$

2. Lattice test conditions a_1, a_2, a_3 3I5/3I5 (2 cards)

b_1, b_2, b_3

e.g. for '1, 0, 1,', h + 1 would be tested.

Two cards are necessary even if the second is blank. Two conditions would be needed for I centering.

3. Modulus for the test, i.e. for h + 1 = 2n, MOD = 2. I5

EXAMPLE OF HKLTRN

```
$*RU HKLTRN[40,32\2\]            INPUT & EXECUTE HKLTRN

ASSIGN FILES ..THEN TYPE CO FOLLOWED BY A CARRIAGERETURN.

AØØ5 ØØ1111
$AS MUØ:AJVUAC.DAT,7
$CO

ENTER TRANSFORMATION MATRIX,LATTICE TEST MATRIX,
AND THE MODULUS OF THE TEST.(DEFAULT=2)
*Ø.5,Ø.Ø,Ø.5,Ø.Ø,1.Ø,Ø.Ø,=.5,Ø.Ø,Ø.5,
*1,Ø,1,
*
*2,

AØØ2 Ø5214Ø
$CO

THE NUMBER OF REFLECTIONS READ IS   332Ø
THE NUMBER OF REFLECTIONS TRANSFORMED AND WRITTEN ON THENEW TAPE IS   1663
```

```
        C         HKLTRN...
        C         PROGRAM TO TRANSFORM H,K,L AND ELIMINATE
        C         LATTICE EXTINCTIONS.
        C
ØØØ1              DIMENSION F(13),T(3,3),LAT(2,3)
ØØØ2              NRIT=1
ØØØ3              NHKLIN=7
ØØØ4              NHKOUT=4
ØØØ5              CALL SETFIL(NRIT,'D',IOERR,'KB')
ØØØ6              CALL SETFIL(NHKLIN,'HKLDAT.DAT',IOERR,'DK',Ø.Ø)
ØØØ7              CALL SETFIL(NHKOUT,'HKLNEW.DAT',IOERR,'DK',Ø.Ø)
ØØØ8              WRITE(NRIT,1)
ØØØ9    1         FORMAT(' ASSIGN FILES ..THEN TYPE CO FOLLOWED BY A CARRIAGE
                  1RETURN.'/)
ØØ1Ø              PAUSE1111
ØØ11              WRITE(6,2)
ØØ12    2         FORMAT(/' ENTER TRANSFORMATION MATRIX,LATTICE TEST MATRIX,'/
                  1 ' AND THE MODULUS OF THE TEST.(DEFAULT=2)'/)
ØØ13              READ(NRIT,#)((T(I,J),J=1,3),I=1,3),((LAT(K,L),L=1,3),K=1,2),IMOD
ØØ14    3         FORMAT(9F8.3/315/315/15)
ØØ15              NRED=Ø
ØØ16              NWRIT=Ø
ØØ17    99        READ(NHKLIN,END=1ØØ) IH,IK,IL,NOT,(F(I),I=1,13)
ØØ18              NRED=NRED+1
ØØ19              ITEST=MOD((IH*LAT(I,1)+IK*LAT(1,2)+IL*LAT(1,3)+
                  1IH*LAT(2,1)+IK*LAT(2,2)+IL*LAT(2,3)),IMOD)
ØØ2Ø              IF(ITEST.EQ.Ø) GO TO 2Ø
ØØ21              GO TO 99
ØØ22    2Ø        FH=IH
ØØ23              FK=IK
ØØ24              FL-IL
ØØ25              FHP=T(1,1)*FH+T(1,2)*FK+T(1,3)*FL
ØØ26              FKP=T(2,1)*FH+T(2,2)*FK+T(2,3)*FL
ØØ27              FLP=T(3,1)*FH+T(3,2)*FK+T(3,3)*FL
ØØ28              IHP=SIGN(1.Ø,FHP)*(ABS(FHP)+Ø.ØØ5)
ØØ29              IKP=SIGN(1.Ø,FKP)*(ABS(FKP)+Ø.ØØ5)
ØØ30              ILP=SIGN(1.Ø,FLP)*(ABS(FLP)+Ø.ØØ5)
ØØ31              WRITE(NHKOUT)IHP,IKP,ILP,NOT,(F(I),I=1,13)
ØØ32              NWRIT=NWRIT+1
ØØ33              GO TO 99
ØØ34    1ØØ       ENDFILE NHKOUT
ØØ35              WRITE(6,4)NRED,NWRIT
ØØ36    4         FORMAT(' THE NUMBER OF REFLECTIONS READ IS',17/
                  1' THE NUMBER OF REFLECTIONS TRANSFORMED AND WRITTEN ON THE
                  2NEW TAPE IS',17/)
ØØ37            END

        ROUTINES CALLED:
        SETFIL, MOD    , SIGN   , ABS

        SWITCHES = /ON

        BLOCK       LENGTH
```

```
MAIN.   877    (ØØ3332)*

**COMPILER ----- CORE**
   PHASE        USED  FREE
DECLARATIVES  ØØ366 Ø55Ø3
EXECUTABLES   ØØ847 Ø5Ø22
ASSEMBLY      Ø151Ø Ø7276
```

PROGRAM: LXEDIT H. L. Carrell

LXEDIT IS A LINE EDITOR FOR FORMATTED PDP 11/40 FILES. IT IS A 1 (ONE) PASS EDITOR AND THE RESULT IS AN UPDATED FILE AS SPECIFIED BY THE USER. THE LINE EDITOR DOES NOT SEARCH FOR TEXT BUT SIMPLY COUNTS LINES AND PERFORMS INSTRUCTION(S) SUPPLIED BY THE USER. THE INSTRUCTIONS ALLOWED ARE DELETE, INSERT, REPLACE AND EXIT. THE INSTRUCTIONS ARE GIVEN AS FOLLOWS:

DELETE

$D(N,M)

$D is punched in cols 1 and 2

N is the sequence number of the first line to be deletec

M is the sequence number of the last line to be deleted

if M=Ø or <N1 then M set equal to N and only 1 line, namely N will be deleted

INSERT

$In,

$I is punched or typed in cols 1 and 2

n the sequence number of the line just before which the trailing cards will be inserted. The current insert instruction is terminated when the next instruction is encountered.

REPLACE

$RN,M,

$R punched in cols 1 and 2

N,M, the lines of sequence number N through and including M will be replaced by the cards following until a new instruction is encountered.

The $RN,M, instruction is equivalent to either:

A. $DN,M,
$IM+1,

or

B. $In,
$DN,M,

The files for the run are specified by the user via the teletype at execution time.

Input edit file, command file <

output file < input edit file, edit instructions file

LISTFC (12/74 version)

The purpose of this program is to produce a compact listing of Fo and Fcalc. The reflection input is that generated by CALCSF and resides on FOURR.DAT. The remainder of the input is entered via the teletype at run time and is self-explanatory. In order to run LISTFC, login on same UIC as FOURR.DAT was produced under. This program resides on disk Ø1, Ø4 (any disk containing CALCSF).

Sample input to LISTFC.

note: CALCSF is run first to produce FOURR.DAT file

```
$*RU LISTFC

LISTFC

STRUCTURE TYPE
1=NON-CENTRIC
2=CENTRIC  *2

WHICH INDEX VARIES FASTEST, H,K, OR L?*L

WHICH INDEX VARIES 2ND FASTEST, H OR K ?*K

$*
```

Sample output from LISTFC

(0, 0)

2	98	102
4	191	-205
6	532	-498
8	164	159
10	284	-279
12	12x	-11
14	308	-319
16	102	97
18	130	119

(0, 2)

0	377	373
2	1069	-1068
4	79	-80
6	123	-112
8	377	383
10	46	50
12	282	283
14	113	-109
16	49	55

(0, 4)

0	462	466
2	42	-41
4	424	432
6	28	-26
8	189	-188
10	315	-320
12	82	89
14	68	-65
16	14x	03

(0, 6)

0	83	-84
2	246	-252
4	63	68
6	57	59
8	19x	00
10	13x	-18
12	185	178
14	31	26

(0, 8)

0	149	149
2	30	23
4	21x	26
6	13x	03
8	32	-31
10	61	-57

(1, 1)

1	568	564
3	465	-468
5	185	-171
7	209	204
9	83	-85
11	116	117
13	124	-130
15	30	-35
17	54	58

(1, 2)

0	559	-581
2	78	-80
4	367	354
6	73	76
8	121	-122
10	75	-75
12	71	74
14	70	75
16	14x	-24

(1, 3)

1	25	-22
3	180	-177
5	56	64
7	95	98
9	142	-139
11	145	147
13	13x	21
15	24	-14
17	24x	-17

(1, 4)

0	63	-64
2	10x	06
4	133	128
6	38	41
8	83	-85
10	79	-75
12	31	26
14	27	31
16	17x	09

(1, 5)

1	45	46
3	43	40
5	141	138
7	14x	-21
9	235	-236
11	17x	16
13	14x	27
15	14x	05

(1, 6)

2	33	-35
4	50	-47
6	18x	07
8	55	55
10	34	40
12	14x	01
14	24x	-16

(1, 7)

1	72	-76
3	80	-81
5	41	44
7	58	58
9	13x	-12
11	74	75

(1, 8)

0	72	68
2	30	28
4	31	-24
6	24	-26
8	16x	12
10	14x	00

(1, 9)

1	82	83
3	17x	00
5	23x	05
7	14x	-14

(2, 0)

0	1297	1280
2	190	-185
4	479	476
6	213	-199
8	25	-21
10	325	-335
12	89	92
14	160	-159
16	52	50

(2, 1)

1	738	-734
3	10x	-17
5	209	204
7	39	43
9	11x	02
11	98	103
13	132	138
15	33	35
17	70	-62

(2, 2)

0	131	132
2	884	-874
4	122	120
6	49	43
8	239	240
10	41	-42
12	254	253
14	76	-74
16	24x	35

(2, 3)

1	42	-44
3	338	337
5	286	269
7	131	-130
9	271	-279
11	86	-83
13	58	63
15	24	17

(2, 4)

0	522	519
2	99	-99
4	172	172
6	11x	-21
8	37	-34
10	193	-192
12	37	45
14	116	-114
16	22x	17

(2, 5)

1	132	-135
3	73	-72
5	12x	01
7	34	41
9	54	51
11	54	62
13	52	39
15	21x	12

(2, 6)

0	37	22
2	185	-186
4	26	-13
6	12x	11
8	58	60
10	20x	19
12	117	108

(2, 7)

1	116	114
3	17x	04
5	55	-55
7	13x	01
9	14x	21
11	39	-31

(2, 8)

0	115	110
2	14x	08
4	26	26
6	13x	10
8	28	-26

(2, 9)

1	14x	09
3	33	-30
5	21x	-27

(3, 1)

1	232	-217
3	10x	03
5	304	295
7	98	82
9	281	-286
11	85	85
13	42	50
15	13x	06
17	44	-37

(3, 2)

0	288	-277
2	133	-124
4	206	189
6	85	80
8	70	-79
10	54	-49
12	89	90
14	48	57
16	28	-30

(3, 3)

1	92	100
3	208	-189
5	10x	02
7	107	99
9	91	-76
11	97	99
13	32	-26

(3, 4)

0	31	13
2	43	53
4	131	130
6	32	-28
8	86	-89
10	84	-83
12	17x	07
14	20x	14

(3, 5)

1	140	143
3	111	-108
5	52	-59
7	63	53
9	28	-14
11	46	36
13	74	-67

(3, 6)

0	14x	-34
2	75	-68
4	40	-45
6	13x	07
8	79	82
10	55	59
12	15x	18

(3, 7)

1	13x	05
3	74	-66
5	21x	00
7	44	42
9	14x	00
11	53	39

(3, 8)

0	94	102
2	42	50
4	13x	07
6	34	-33
8	14x	09

(3, 9)

1	14x	18
3	14x	00
5	30	23

(4, 0)

0	150	186
2	320	-309
4	437	436
6	60	34
8	141	-149
10	247	-252
12	210	217
14	13x	00
16	14x	-11

(4, 1)

1	330	-318
3	230	-234
5	10x	-30
7	115	110
9	141	146
11	127	134
13	65	66
15	13x	09

(4, 2)

0	178	175
2	322	-309
4	182	189
6	29	00
8	12x	12
10	114	-115
12	157	158
14	39	-43
16	14x	11

(4, 3)

1	260	266
3	148	145
5	11x	08
7	89	-84
9	108	-108
11	91	-87
13	70	-69
15	24x	-22

(4, 4)

0	362	360
2	106	-97
4	55	-51
6	48	-59
8	85	91
10	25	-23
12	24	23
14	115	-109

(4, 5)

1	133	-141
3	87	-78
5	34	-30
7	38	46
9	87	84
11	81	74
13	38	36

(4, 6)

0	166	165
2	76	-72
4	64	-70
6	20x	-18
8	60	65
10	19x	14
12	37	26

(4, 7)

1	74	75
3	49	54
5	13x	10
7	28	-21
9	54	-46

(4, 8)

0	48	48
2	14x	-15
4	26	15
6	22x	13
8	18x	-15

(4, 9)

1	36	-39

(5, 1)

1	39	-43
3	41	-32
5	139	125
7	29	22
9	178	-170
11	88	79
13	44	48
15	20x	-12

(5, 2)

0	142	134
2	25	-19
4	131	-134
6	66	-68
8	116	123
10	78	84
12	14x	-26
14	68	-57

(5, 3)

1	122	112
3	67	-53
5	35	-25
7	13x	17
9	71	-62
11	59	41
13	27	-26
15	15x	-16

(5, 4)

0	153	155
2	39	44
4	28	-33
6	66	-61
8	24	23
10	13x	-10
12	31	-40
14	44	-38

(5, 5)

1	53	53
3	96	-102
5	31	-38
7	63	57
9	17x	18
11	43	40
13	33	-31

(5, 6)

0	68	-83
2	67	-63
4	21x	21
6	14x	10
8	33	29
10	14x	15

(5, 7)

1	39	47
3	14x	-21
5	13x	03
7	20x	08
9	37	-33

(5, 8)

0	24	21
2	21x	30
4	48	46
6	15x	08

(6, 0)

0	129	107
2	202	-199
4	15x	08
6	20x	-17
8	56	73
10	26	19
12	120	117
14	56	-48

(6, 1)

1	80	-83
3	137	-137
5	99	-102
7	77	75
9	154	156
11	80	72
13	20x	09

(6, 2)

0	273	249
2	22x	-32
4	53	64
6	22x	-23
8	38	-25
10	86	-93
12	31	28
14	71	-64

(6, 3)

3	12x	11
5	103	-105
7	18x	09
9	27	26
11	61	-62
13	109	-108

(6, 4)

0	46	19
2	123	-129
4	13x	04
6	31	26
8	20x	39
10	15x	07
12	76	67

(6, 5)

1	80	-81
3	55	-58
5	19x	-16
7	34	38
9	49	52
11	53	44

(6, 6)

0	81	82
2	23	07
4	29	26
6	22x	09
8	27	-22
10	58	-47

(6, 7)

1	21x	15
3	61	61
5	47	40
7	30	-26

(6, 8)

0	23x	06
2	42	-29

(7, 1)

1	75	65
3	103	-94
5	51	-53
7	51	51
9	14x	30
11	54	43
13	52	-47

(7, 2)

0	82	71
2	12x	05
4	65	-61
6	34	-26
8	65	64
10	21x	26
12	14x	-29

(7, 3)

1	42	41
3	31	-11
5	31	33
7	13x	03
9	83	-76
11	15x	05

(7, 4)

0	56	53
2	13x	04
4	13x	-16
6	25	-21
8	23x	23
10	14x	04

(7, 5)

1	68	-76
3	32	-21
5	71	62
7	34	26
9	57	-39

(7, 6)

0	32	-32
2	32	-20
4	29	21
6	14x	03
8	15x	03

(7, 7)

1	23x	31
3	17x	15
5	28	20

(8, 0)

0	81	65
2	119	-116
4	123	-118
6	14x	-14
8	122	126
10	89	82
12	36	33

(8, 1)

1	36	-33
3	13x	-18
5	12x	04
7	25	14
9	26	07
11	14x	07

(8, 2)

0	195	181
2	32	36
4	17x	14
6	13x	-16
8	28	-23
10	66	-62

(8, 3)

1	16x	13
3	22x	22
5	28	14
7	13x	02
9	32	-25

(8, 4)

0	84	-88
2	102	-98
4	34	29
6	55	41
8	16x	01

(8, 5)

1	34	-27
3	14x	06
5	16x	01
7	18x	05

(8, 6)

0	42	34
2	14x	16
4	57	51

(9, 1)

1	29	29
3	57	-46
5	13x	-18
7	34	28
9	14x	09

(9, 2)

0	49	-43
2	13x	06
4	55	53
6	21x	19
8	36	-35

(9, 3)

1	23x	20
3	13x	02
5	15x	15
7	14x	07

(9, 4)

0	28	-39
2	16x	-16
4	34	27
6	20x	08

(9, 5)

1	43	-35
3	24x	-11

(10, 0)

0	15x	-36
2	66	-60
4	14x	09
6	35	23

(10, 1)

1	14x	01
3	29	32
5	31	26

(10, 2)

0	68	63
2	17x	24
4	15x	22
6	14x	00

(10, 3)

1	55	-51

PROGRAM NAME	MSRED
PURPOSE	calculates structure amplitudes from raw data
LIMITATIONS	
SWITCH SETTINGS	
LOGICAL UNITS	6 KB input for item number 11 1 all other input information
FILE ASSIGNMENTS	1 may either be assigned to CR or DKO

MSRED

All input except (1) can be typed on cards either formatted as specified or unformatted and with entries separated by commas with no blanks. (1) is entered from the teletype when the program calls for KB input.

1. TITLE Columns 1-60 (15A4)

2. CELL CARD $a, b, c, \alpha, \beta, \gamma, \lambda$ (7F10.5)

3. ORIENTATION MATRIX from the diffractometer. (3F10.5) 3 cards

4. NDECAY, NABS, NLP, NBACK (4I5)

   NDECAY Application of decay correction for crystal stability and type of correction (=0,1,2...). See 7. below.

   NABS Application of absorption correction and type (=0,1,2...). See 9. below.

   NLP Will monochromator two theta LP correction be applied and read 1=yes, 0=no.

   NBACK Application of background correction and type. (=0,1,2...) See 8. below.

5. Two-theta monochromator (If NLP=1) (F10.3)

6. CUTOFF, SIGM (2F10.5 ~~I5,F10.6~~)

   CUTOFF = ~~an integer, n~~. n x sigma = cutoff for "unobserved" reflections

   SIGM = ESD for decay correction (usually 0.022)

7. AD(I), depending on NDECAY value. Read <u>if</u> NDECAY > 0.

   (a)* AD(1), AD(2), AD(3) (only if NDECAY = 1) (3F10.5)

   coefficients for correction for decay

   $CORR = AD(1) + AD(2) \cdot T + AD(3) \cdot T^2$ where T = exposure time in hours.

   (b) (AD(I), AT(I), I = 1, NDECAY) (8F10.5)

   points in the decay correction curve

   AD(I) correction factor at time AT(I)

   this read only if NDECAY ≥ 2

   a maximum of 100 points allowed

MSRED

8. Background Correction Cards. This card only appears if NBACK > 0.

   (a)* BT - peak to background time ratio read if NBACK ≥ 1 (F10.5)

   (b) THB(II), BGD(I), I=1, NBACK NBACK ≥ 2 (8F10.5)

   THB - 2θ

   BDG - background

   30 points maximum currently

9. Absorption Correction Cards (only if NABS ≥ 1)

   (a) ellipsoid of revolution (NABS = 1)

   (b) curve A(φ) (NABS > 1)

10. Specifications for eliminating space group systematically absent reflections.

   (a) ICELL (I5)
   (lattice type specification)

   1 - P; 2 - A; 3 - B; 4 - C; 5 - I; 6 - F.

   (b) IGR, IHT, IKT, ILT, IMOD (5I5)

   up to 7 of these cards are read.

   If less then 7 are to be read, a blank card will terminate the reading of the cards.

   IGR is the reflection class

class	HKL	OKL	HOL	HKO	HOO	OKO	OOL
IGR	1	2	3	4	5	6	7

class NY.

The test is performed in the following manner.

IT = MOD (IHT·h + IKT·k + ILT·ℓ, IMOD)

1 ≡ Allowed
0 ≡ NOT Allowed.

if IT = 0 then reflection is allowed by symmetry

≠ 0 " is not allowed by symmetry

Tests are performed only on the reflection groups specified.

Thus if space group is $P2_1/c$

where absences are

h 0 ℓ ℓ = 2n + 1

0 k 0 $k = 2n + 1$

0 0 1 $\ell = 2n + 1$

The following 4 cards would be used

IGR	ITH	ITK	ILT	IMOD
3	1	0	1	2
6	0	1	0	2
7	0	0	1	2

ICELL = 1

11. IFRST, ILST, ISKP (3I5)

DATA LIMIT SPECIFICATION

IFRST

This entry allows the user to specify the data which is to be read from the raw data tape for reduction. This is done because of the problems which arise during data collection which allow the recording of unwanted or even "garbage" data. By the careful use of this entry, the data may be culled for the desirable data so that later painful elimination of meaningless data may be avoided. If the user is so fortunate that the data collection went without error, the input here is

IFRST = first sequence number on the tape

ILST = last sequence number on the tape

ISKP = 0

A second card with IFRST ≤ 0 will then terminate the data reduction.

12. NTABL number of structure factor tables (I5)

13. FMT format for f-table cards (15A4)

14. f tables in the format specified. There must be 21 values/table with sin θ/λ up to 1.2.

MSRED

Sample output of data reduction:

```
1***RAW DATA    CESSOR***

     AJV-UAC

 DATE  14-MAY-74              TIME  11:54:24
1      PRELIMINARY INPUT FOR DATA REDUCTION
  FOR...AJV-UAC

**DIRECT CELL PARAMETERS**
 A= 10.1710    ALPHA=  99.86   COS(ALPHA)=-0.17124   SIN(ALPHA)= 0.98523
 B= 12.0990    BETA =  93.40   COS(BETA) =-0.05931   SIN(BETA) = 0.99824
 C=  5.6710    GAMMA=  91.47   COS(GAMMA)=-0.02565   SIN(GAMMA)= 0.99967
 VOLUME=     805.84 CUBIC ANGSTROMS.

 **RECIPROCAL CELL PARAMETERS**
 A*=0.09856  ALPHA*=  80.03  COS(ALPHA*)= 0.17312  SIN(ALPHA*)= 0.98490
 B*=0.08395  BETA* =  86.29  COS(BETA*) = 0.06468  SIN(BETA*) = 0.99791
 C*=0.15247  GAMMA*=  87.91  COS(GAMMA*)= 0.03641  SIN(GAMMA*)= 0.99934
 VOLUME*= 0.001239401 /CUBIC ANGSTROM.

 WAVELENGTH = 1.54180 ANGSTROMS.
 THE COEFFICIENTS FOR THE CALCULATION OF SIN(THETA)**2/LAMBDA**2
 IN THE EQUATION
 SSQ=S1*H*H+S2*K*K+S3*L*L+S4*H*K+S5*H*L+S6*K*L   ARE
 S1= 0.00342839      S2= 0.00176174      S3= 0.00581171
 S4= 0.00015062      S5= 0.00048594      S6= 0.00110793

 **ORIENTATION MATRIX**
   0.03257   -0.08097   -0.06336
   0.09797    0.00287    0.02606
  -0.01041   -0.02195    0.13621


 P1(BAR) DATA..2-THETA(MONOCHROMATOR)=26.30DEG.

 DATA WITH I(MEAS) >  0.00*SIGMA(I) WILL BE CONSIDERED OBSERVED.
    0.0220 IS THE INSTRUMENTAL STABILITY CONSTANT.

 NO BACKGROUND TO BE SUBTRACTED.
 NO ABSORPTION CORRECTION.

 LATTICE TYPE IS  1

 NO TESTS FOR SPACE GROUP ABSENCES ARE TO BE MADE.


 PRELIMINARY INPUT COMPLETE.


 DATE  14-MAY-74              TIME  11:54:31

 **DATA REDUCTION **
 FOR...AJV-UAC

   IFRST=    1   ILST=  422   ISKP=    0
```

PROGRAM NAME	PARAML
PURPOSE	produces a compact listing of final atomic parameters
LIMITATIONS	100 atoms
SWITCH SETTINGS	all switches down
LOGICAL UNITS	1 all input (control statements and parameters)
FILE ASSIGNMENTS	1 should be assigned whether CR:, MTØ:, or DKØ:

PARAML

Program Description

This program creates a compact listing of all final atomic parameters of a given compound containing as many as 100 atoms. The atomic coordinates and temperature factors are listed as shown in the sample output. Only 2 characters can be listed as E.S.D. values so care should be taken in determining the NX and NH values on the third input card.

Input Description

The following data should be set up in advance of run on a deck of cards or magnetic tape. All input MUST be entered via the same device, which is assigned logical unit 1.

Ø26 CARD

1) TITLE 60 Alphanumeric characters (10A6)

2) ASTAR, BSTAR, CSTAR (3F10.5)

Astar, Bstar, and Cstar are the a^*, b^*, and c^* reciprocal cell axes respectively. The last page of this program description gives a summary of reciprocal cell relations.

3) NTP, NAT, NAN, NX, NH (3I5, 13I2)

NTP = format for the input atomic parameters

1 = UCLA format (3F10.5, 40X, A6) atom label last on card

2 = XRAY format (7X, A6, 3F8.5) atom label first on card

NOTE: UCLA FORMAT MUST BE USED IF ANY ISOTROPIC ATOMS ARE INPUT.

NAT = total number of atoms to be included in the parameter listing

NAN = number of atoms with anisotropic temperature factors

NX (9I2) = the exponent of the factor 10^{NX} which multiplies the anisotropic atomic parameters to obtain the corresponding list values.

a) The first 3 fields contain the value of NX to be applied to the anisotropic x, y, z coordinates and their E.S.D.s respectively in the following equation:

(fractional x, y, and z coordinates and E.S.D.s)*10^{NX} = listed values

b) The remaining 6 fields of NX values contain the value of NX to be applied to the E.S.D.s of anisotropic temperature factors B_{11}, B_{22}, B_{33}, B_{12}, B_{13}, and B_{23} respectively, as in the following example:

(input B_{11} value)* 4.0/(ASTAR)**2 = listed B_{11}value

(input B_{11} E.S.D. value)*(4.0/(ASTAR)**2)*10^{NX} = listed B_{11}E.S.D.

NH (4I2) = the exponent of the factor 10^{NH} which multiplies the isotropic atomic parameters to obtain the corresponding list values.

a) The first 3 fields contain the value of NH to be applied to the isotropic x, y, z coordinates and their respective E.S.D.s. The calculation is exactly the same as in NX a) with 10^{NH} replacing 10^{NX}.

b) The remaining field contains the value of NH to be applied to the E.S.D. of the isotropic temperature factor B of each isotropic atom as follows:

input B value = listed B value

(input B E.S.D. value)*10^{NH} = listed value

NOTE: Incorrect values in the NX and NH fields is the most common source of error in this program. A hand calculation of the given examples for a typical B_{11} and its E.S.D. and an isotropic B E.S.D. will ensure a proper selection of NX and NH values. A typical NX field is 4 4 4 222222 and a typical NH field is 3331. (1 blank between each number)

4) Anisotropic coordinates and temperature factors.

Two cards are read for each anisotropic atom input (NAN). The first card contains the x, y, z coordinates; [UCLA(NTP=1)=(3F10.5, 40X, A6) or XRAY(NTP=2)=(7X, A6, 3F8.5)].

The second card ontains the anisotropic temperature factors; [UCLA=(6F10.5, 10X, A6) or XRAY=(13X, 6F8.5)].

5) Isotropic coordinates and temperature factors.

NTP MUST BE 1 IF ANY ISOTROPIC ATOMS ARE INPUT.

One card in the UCLA format (4F10.5, 30X, A6) containing the x, y, z coordinates and isotropic temperature factor is read for each isotropic atom input (NAT-NAN). The isotropic atoms follow the last anisotropic atom input.

6) Anisotropic coordinate and temperature factor E.S.D.s

Two cards are read for each anisotropic atom input. The first card contains the coordinate E.S.D.s (3F10.5), and the second card contains the temperature factor E.S.D.s (6F10.5).

7) Isotropic coordinate and temperature factor E.S.D.s

One card is read for each atom input (3F10.5, F10.3). As mentioned in 5) NTP MUST EQUAL 1 if isotropic atoms are included.

EOF CARD

BLANK CARD

PARAML

SUMMARY OF ANISOTROPIC TEMPERATURE FACTOR CONVERSIONS

C = 1.0 for XRAY format input; C = 2.0 for UCLA format input

Input temp. factor		Listed temp. factor
B_{11}	*4.0/(ASTAR)**2=	B_{11}
B_{22}	*4.0/(BSTAR)**2=	B_{22}
B_{33}	*4.0/(CSTAR)**2=	B_{33}
B_{12}	*4.0/C*ASTAR*BSTAR=	B_{12}
B_{13}	*4.0/C*ASTAR*CSTAR=	B_{13}
B_{23}	*4.0/C*BSTAR*CSTAR=	B_{23}

TABLE 20

Collection of Relations for Triclinic Reciprocal Cell Elements

$$a^* = \frac{bc \sin \alpha}{V} \cdot \lambda \tag{51}$$

$$b^* = \frac{ac \sin \beta}{V} \cdot \lambda \tag{52}$$

$$c^* = \frac{ab \sin \gamma}{V} \cdot \lambda \tag{53}$$

ORTHO- RHOMBIC MONO- CLINIC TRI- CLINIC

$$a^* = \frac{1 \cdot \lambda}{a \sin \beta^* \sin \gamma} = \frac{1 \cdot \lambda}{a \sin \beta \sin \gamma^*} \tag{54}$$

a^* $1/a$ $1/a \sin\beta$ $1/a \sin\beta \sin\gamma^*$

$$b^* = \frac{1 \cdot \lambda}{b \sin \alpha^* \sin \gamma} = \frac{1 \cdot \lambda}{b \sin \alpha \sin \gamma^*} \tag{55}$$

b^* $1/b$ $1/b$ $1/b \sin\alpha \sin\gamma^*$

$$c^* = \frac{1 \cdot \lambda}{c \sin \alpha^* \sin \beta} = \frac{1 \cdot \lambda}{c \sin \alpha \sin \beta^*} \tag{56}$$

c^* $1/c$ $1/c \sin\beta$ $1/c \sin\alpha \sin\beta^*$

$$a^* : b^* : c^* = \frac{\sin \alpha}{a} : \frac{\sin \beta}{b} : \frac{\sin \gamma}{c}. \tag{68}$$

$$V^* = a^*b^*c^*\sqrt{1 - \cos^2 \alpha^* - \cos^2 \beta^* - \cos^2 \gamma^* + 2 \cos \alpha^* \cos \beta^* \cos \gamma^*}. \quad (12), (23)$$

$$V^* = a^*b^*c^* \sin \alpha^* \sin \beta^* \sin \gamma. \tag{48}$$

$$= a^*b^*c^* \sin \alpha^* \sin \beta \sin \gamma^* \tag{49}$$

$$= a^*b^*c^* \sin \alpha \sin \beta^* \sin \gamma^* \tag{50}$$

$$V^* = \frac{1}{V} \cdot \lambda^3 \quad (61), (64)$$

$$\cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}. \tag{31}$$

$$\cos \beta^* = \frac{\cos \alpha \cos \gamma - \cos \beta}{\sin \alpha \sin \gamma}. \tag{32}$$

$$\cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}. \tag{33}$$

$$\cot \frac{\alpha^*}{2} = \sqrt{\frac{\sin (\sigma - \beta) \sin (\sigma - \gamma)}{\sin \sigma \sin (\sigma - \alpha)}}, \tag{37}$$

$$\cot \frac{\beta^*}{2} = \sqrt{\frac{\sin (\sigma - \alpha) \sin (\sigma - \gamma)}{\sin \sigma \sin (\sigma - \beta)}}, \tag{38}$$

$$\cot \frac{\gamma^*}{2} = \sqrt{\frac{\sin (\sigma - \alpha) \sin (\sigma - \beta)}{\sin \sigma \sin (\sigma - \gamma)}}, \tag{39}$$

$$\text{where } \sigma = \frac{\alpha + \beta + \gamma}{2}.$$

$$\frac{\sin \alpha^*}{\sin \alpha} = \frac{\sin \beta^*}{\sin \beta} = \frac{\sin \gamma^*}{\sin \gamma}. \tag{70}$$

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TABLE 21

Collection of Relations for Triclinic Direct Cell Elements

$$a = \frac{b^*c^* \sin \alpha^*}{V^*} \cdot \lambda \tag{51'}$$

$$b = \frac{a^*c^* \sin \beta^*}{V^*} \cdot \lambda \tag{52'}$$

$$c = \frac{a^*b^* \sin \gamma^*}{V^*} \cdot \lambda \tag{53'}$$

$$a = \frac{1 \cdot \lambda}{a^* \sin \beta \sin \gamma^*} = \frac{1 \cdot \lambda}{a^* \sin \beta^* \sin \gamma}. \tag{54'}$$

$$b = \frac{1 \cdot \lambda}{b^* \sin \alpha \sin \gamma^*} = \frac{1 \cdot \lambda}{b^* \sin \alpha^* \sin \gamma}. \tag{55'}$$

$$c = \frac{1 \cdot \lambda}{c^* \sin \alpha \sin \beta^*} = \frac{1 \cdot \lambda}{c^* \sin \alpha^* \sin \beta}. \tag{56'}$$

$$a : b : c = \frac{\sin \alpha^*}{a^*} : \frac{\sin \beta^*}{b^*} : \frac{\sin \gamma^*}{c^*}. \tag{68'}$$

$$V = abc\sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}. \quad (12'), (23')$$

$$V = abc \sin \alpha \sin \beta \sin \gamma^* \tag{48'}$$

$$= abc \sin \alpha \sin \beta^* \sin \gamma \tag{49'}$$

$$= abc \sin \alpha^* \sin \beta \sin \gamma. \tag{50'}$$

$$V = \frac{1}{V^*} \quad (61'), (64')$$

$$\cos \alpha = \frac{\cos \beta^* \cos \gamma^* - \cos \alpha^*}{\sin \beta^* \sin \gamma^*}. \tag{31'}$$

$$\cos \beta = \frac{\cos \alpha^* \cos \gamma^* - \cos \beta^*}{\sin \alpha^* \sin \gamma^*}. \tag{32'}$$

$$\cos \gamma = \frac{\cos \alpha^* \cos \beta^* - \cos \gamma^*}{\sin \alpha^* \sin \beta^*}. \tag{33'}$$

$$\cot \frac{\alpha}{2} = \sqrt{\frac{\sin (\sigma^* - \beta^*) \sin (\sigma^* - \gamma^*)}{\sin \sigma^* \sin (\sigma^* - \alpha^*)}}. \tag{37'}$$

$$\cot \frac{\beta}{2} = \sqrt{\frac{\sin (\sigma^* - \alpha^*) \sin (\sigma^* - \gamma^*)}{\sin \sigma^* \sin (\sigma^* - \beta^*)}}. \tag{38'}$$

$$\cot \frac{\gamma}{2} = \sqrt{\frac{\sin (\sigma^* - \alpha^*) \sin (\sigma^* - \beta^*)}{\sin \sigma^* \sin (\sigma^* - \gamma^*)}}, \tag{39'}$$

$$\text{where } \sigma^* = \frac{\alpha^* + \beta^* + \gamma^*}{2}.$$

$$\frac{\sin \alpha}{\sin \alpha^*} = \frac{\sin \beta}{\sin \beta^*} = \frac{\sin \gamma}{\sin \gamma^*}. \tag{70'}$$

Sample of Paraml KB: Input

```
TIME:-10:01:44
CRYSNET 20-APR-74
DOS V08-08
$*LO 40,2
DATE:-24-SEP-74
TIME:-10:04:01
$*AS CR:,1
$*RU PARAML
$*↑C
.*FI
```

cards read here

Note that no output device is assigned. After all cards are read, parameter list is printed on LP:

PARAML PROGRAM IS ON DISK Ø4
UNDER UIC 4Ø,2

```
*****************************************************************************
*                                                                           *
*                          PARAMETER LISTING                                *
*                                                                           *
*                                 FOR                                       *
*        CTA FINAL COORDINATES 9/9/74                                       *
*                                                                           *
*****************************************************************************
```

FOR THE 16 ANISOTROPIC ATOMS THE FOLLOWING APPLY:
X MULTIPLIED BY 10** 4
Y MULTIPLIED BY 10** 4
Z MULTIPLIED BY 10** 4

FOR THE 16 REMAINING ATOMS THE FOLLOWING APPLY:
X MULTIPLIED BY 10** 3
Y MULTIPLIED BY 10** 3
Z MULTIPLIED BY 10** 3

	X	Y	Z	B11	B22	B33	B12	B13	B23
1	-1745(6)	2116(3)	5710(0)	5.70(26)	3.03(16)	3.03(19)	-0.12(17)	-0.44(23)	-0.24(18)
1	-18(6)	3341(3)	8821(5)	9.33(31)	4.12(17)	3.07(18)	-1.01(22)	-0.75(21)	0.00(16)
2	-777(5)	1833(3)	8525(6)	6.78(24)	3.42(15)	3.64(18)	-0.23(19)	-0.79(20)	0.63(15)
3	785(6)	3606(3)	1557(6)	7.43(28)	4.96(19)	3.47(18)	-1.96(22)	0.31(20)	0.78(17)
4	-1021(6)	2801(3)	2696(6)	5.89(22)	6.22(22)	3.35(18)	-1.54(20)	-0.03(19)	-0.37(20)
5	878(6)	1356(3)	905(7)	9.48(31)	2.44(13)	5.64(23)	0.39(18)	-2.03(28)	0.37(18)
6	687(6)	-197(3)	485(6)	8.37(31)	2.90(15)	4.87(24)	0.01(18)	-0.49(23)	0.21(17)
1	-650(7)	2824(4)	6287(7)	5.16(31)	2.50(19)	2.64(23)	-0.20(22)	-0.40(24)	0.02(17)
2	824(8)	2668(4)	5477(8)	5.50(36)	4.08(24)	2.97(25)	0.19(27)	0.03(24)	0.09(22)
3	956(9)	3468(6)	4260(11)	5.89(41)	5.37(34)	4.94(35)	-0.58(32)	1.22(33)	0.55(31)
4	146(11)	4273(5)	5030(12)	9.47(56)	4.59(34)	6.04(43)	-0.35(37)	1.18(48)	0.63(32)
5	-1120(8)	3856(4)	5875(9)	6.54(37)	2.94(20)	3.72(28)	0.33(25)	-0.40(31)	0.20(24)
6	-480(8)	2653(4)	8043(9)	5.22(34)	2.88(22)	3.08(28)	0.24(23)	-0.05(26)	0.01(22)
7	153(11)	3271(6)	2751(10)	6.94(44)	5.76(39)	2.98(30)	-0.94(37)	-0.14(35)	0.19(32)
8	1167(9)	453(5)	1212(9)	6.24(38)	3.40(23)	3.30(30)	0.18(27)	0.57(29)	0.43(23)
9	2184(10)	355(5)	2541(12)	8.10(49)	3.98(26)	5.26(41)	0.17(33)	-1.19(41)	0.53(28)

	X	Y	Z	B
1N	-269(9)	232(4)	634(8)	9.2(16)
2N	-168(8)	220(5)	454(10)	4.7(17)
3N	-129(7)	150(4)	594(10)	5.8(17)
3A	59(17)	318(11)	90(22)	12.8(39)
3B	-44(25)	359(15)	2(31)	14.1(61)
21	171(7)	271(4)	630(9)	3.5(17)
22	74(8)	193(5)	495(9)	8.1(17)
31	197(7)	363(5)	413(9)	4.8(20)
41	-18(9)	487(5)	429(9)	6.5(17)
42	92(7)	456(5)	586(12)	12.2(17)
51	-107(8)	399(5)	702(11)	5.9(17)
52	-190(7)	389(5)	518(10)	2.5(19)
85	14(8)	148(5)	0(11)	7.0(18)
91	242(9)	-25(4)	269(9)	7.6(16)
92	264(9)	84(5)	272(10)	12.4(20)
93	162(9)	46(6)	361(11)	9.6(18)

PROGRAM NAME	PECKER
PURPOSE	TO PICK OUT AND LIST THOSE PEAKS FROM A PREVIOUSLY RUN FOURIER EQUAL TO OR GREATER THAN A GIVEN RHO VALUE.
LIMITATIONS	A MAXIMUM OF 600 PEAKS MAY BE FOUND
SWITCH SETTINGS	NONE
LOGICAL UNITS	1 output file of PECKER (PEAKER.DAT) DKØ: 2 input file (from FOURR) CONTUR.DAT, DKØ: 5 printed output file of PECKER; default LP:
FILE ASSIGNMENTS	1 and 2 MUST BE ASSIGNED as follows: AS DKØ:PEAKER.DAT, 1 AS DKØ:CONTUR.DAT, 2
LOCATION OF PROGRAM	DISK Ø1 (on any disk containing the FOURR program)

PECKER (12/74 version)

This is a program which searches the CONTUR.DAT file of a previously run FOURR program for those peaks equal to or greater than a specified rho value. The output consists of a list of the found peaks in order of decreasing rho magnitude. The grid coordinates and the fractional coordinates of the found peaks are listed.

NOTE: The FOURR program must be run first and the file CONTUR.DAT must be created as specified on the 2nd control card in the FOURR program. CONTUR.DAT will overwrite a previously produced CONTUR.DAT file on a disk under the same UIC. CONTUR.DAT is the file searched by PECKER to find the peaks written on PEAKER.DAT and printed on the line printer. PEAKER.DAT and FOURR.DAT (input file to FOURR program) must be deleted from the disk after PECKER is run.

Sample input to Pecker

```
PASS: 1
PASS: 2
PASS: 3
PASS: 4
PASS: 5
PASS: 6
```

end of FOURR run

```
$*AS DK0:PEAKER.DAT,1
$*AS DK0:CONTUR.DAT,2
$*FU PECKER

FOURIER PEAK SEARCH.
RHO(MINIMUM) FOR THE SEARCH IS?*20,

AXIS ORIENTATION IN MAP.
(X=1; Y=2; Z=3)
PAGE TO PAGE AXIS(1,2, OR 3)?*3

 VERTICAL AXIS(DOWN THE PAGE)(1,2, OR 3)?*1

PAGE TO PAGE AXIS IS  Z
VERTICAL AXIS IS  X
HORIZONTAL AXIS IS  Y
$*FU FIP
FIP  24-APR-74
@*FOURR.DAT,PEAKER.DAT/DE
```

from FOURR

comma must be here

axis orientation should be the same as in FOURR map

Sample output from Picker

(this is PEAKER.DAT file)

**** FOURIER PEAK SEARCH ****

ONLY THOSE PEAKS WITH DENSITY GREATER THAN 20 WILL BE PICKED

GRID SETUP OF MAP

	NO.	START	CALC	DELTA
PAGE TO PAGE	60	0	31	1
VERTICAL	60	0	31	1
HORIZONTAL	60	0	31	1

LIST OF THE MAXIMA AND THEIR COORDINATES (UNREFINED)

NO.	GRIDX	GRIDY	GRIDZ	X	Y	Z	RHO
1	12	15	17	0.200	0.250	0.283	66
2	8	15	6	0.133	0.250	0.100	55
3	5	16	10	0.083	0.267	0.167	45
4	7	13	16	0.117	0.217	0.267	36
5	9	17	14	0.150	0.283	0.233	29
6	21	15	29	0.350	0.250	0.483	29
7	4	16	14	0.067	0.267	0.233	27
8	7	13	11	0.117	0.217	0.183	26
9	9	18	21	0.150	0.300	0.350	26
10	11	15	11	0.183	0.250	0.183	25
11	5	10	17	0.083	0.167	0.283	24
12	8	14	23	0.133	0.233	0.383	24
13	7	16	18	0.117	0.267	0.300	23
14	9	15	0	0.150	0.250	0.000	22
15	29	15	11	0.483	0.250	0.183	22
16	3	17	18	0.050	0.283	0.300	22
17	22	4	2	0.367	0.067	0.033	21
18	22	5	2	0.367	0.083	0.033	21
19	4	16	23	0.067	0.267	0.383	21
20	7	13	3	0.117	0.217	0.050	20
21	15	15	14	0.250	0.250	0.233	20
22	26	15	14	0.433	0.250	0.233	20
23	22	14	22	0.367	0.233	0.367	20
24	22	15	22	0.367	0.250	0.367	20

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PRJCTN - 02/14/76

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

DEC PDP-11/40 + VG 3D2
DEC DOS/BATCH 9-20C + VG FDP 6

DESCRIPTION

PRJCTN IS A PROGRAM FOR DISPLAY OF MOLECULES AS STICK BOND FIGURES ALLOWING FOR INTERACTIVE ROTATION ABOUT AXES. IT WAS WRITTEN BY L. MCCANDLISH AT THE UNIVERSITY OF WASHINGTON IN MAY OF 1972 FOR THE CDC 6400 AND CALCOMP PLOTTER. IT WAS MODIFIED SEVERAL TIMES BY L. ANDREWS AT U.W. AND BY L. ANDREWS AND H. BERNSTEIN AT BROOKHAVEN NATIONAL LABORATORY. THE PROGRAM INCLUDES PLOTTING AND MOLECULAR GEOMETRY COMMANDS.

PURPOSE

DISPLAYS MOLECULES AS STICK BOND FIGURES.

LIMITATIONS

690 ATOMS
874 BONDS
50 RANGE (RNGE) COMMANDS
24 SYMMETRY (SYMT) OPERATIONS

THE COUNT OF ATOMS INCLUDES THOSE GENERATED BY SYMMETRY OPERATIONS. EACH RANGE COMMAND REDUCES THE NUMBER OF BONDS ALLOWED BY ONE. THE LATTICE COMMAND ALLOWS ALL SPACE GROUPS TO BE HANDLED WITHIN THE LIMIT OF 24 SYMMETRY OPERATIONS.

SWITCH SETTINGS

13 UP - LIST BOND LENGTHS AS THEY ARE COMPUTED DURING SETUP OF DISPLAY
14 UP - DISPLAY CIRCLES IF SELECTED

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DIAL FUNCTIONS

```
 1  Y-AXIS EULER ANGLE (APPLIED LAST)
 2  X-AXIS EULER ANGLE (APPLIED FIRST)
 3  Z-AXIS EULER ANGLE (APPLIED SECOND)
 4  INTENSITY OFFSET
 5  INTENSITY SCALE
 6  ROTATION RATE
          SWITCHED OFF OR ON BY CARRIAGE RETURN
10  STEREO DISPLAY
          CENTRAL REGION - SINGLE IMAGE
          TO RIGHT - RIGHT-LEFT STEREO
          TO LEFT - UP-DOWN STEREO
```

THE Y-AXIS IS VERTICAL ON THE SCREEN. THE X-AXIS RUNS HORIZONTALLY. THE Z-AXIS IS PERPENDICULAR TO THE SCREEN. THE INTENSITY OFFSET ACTS SOMEWHAT LIKE A BRIGHTNESS CONTROL, WHILE INTENSITY SCALE WORKS LIKE A CONTRAST CONTROL. A NEGATIVE SCALE (CCW) WILL ALLOW THE INTENSITY OFFSET TO CONTROL A CUTOFF PLANE IN THE Z-DIRECTION.

LOGICAL UNITS

```
1        READ COMMAND INPUT FILE
4        KEYBOARD INPUT (DEFAULT KB:)
5        KEYBOARD OUTPUT (DEFAULT KB:)
7        PLOT UNIT (DEFAULT VP:)
```

THERE IS NO VALUE TO THE USER IN DOING ASSIGNMENTS OF THE LOGICAL UNITS. ON THE CONTRARY, THIS CAN CAUSE INEXPLICABLE FAILURES OF THE PROGRAM. THIS INFORMATION IS INCLUDED ONLY TO FACILITATE TRACING LISTINGS.

INTRODUCTION

PRJCTN IS AN INTERACTIVE PROGRAM TO DISPLAY MOLECULES AS STICK BOND FIGURES, ROTATE THE FIGURES, OBTAIN GEOMETRY CALCULATIONS, AND PLOT THE DISPLAYED IMAGE.

INPUT TO THE PROGRAM MAY COME FROM THE KEYBOARD, OR FROM A VARIETY OF SYSTEM DEVICES. SOME OF THE OUTPUT MAY BE SIMILARLY DIRECTED.

THE PROGRAM WORKS IN TWO MAJOR PHASES. FIRST COORDINATES, CELL INFORMATION, SYMMETRY, AND OTHER IMAGE DEFINING COMMANDS ARE READ IN, LARGELY IN AN ORDER-INDEPENDENT FORM. THE MOLECULAR IMAGE FORMED FROM THESE ITEMS IS THEN PASSED ON TO THE SECOND PHASE OF THE PROGRAM, WHICH DISPLAYS THAT IMAGE AND ALLOWS THE USER TO CONTROL ITS ORIENTATION, ROTATION RATE, AND TO SWITCH FROM SINGLE TO STEREO VIEWS. THE USER MAY DO SOME LIMITED EDITING OF THE DISPLAYED IMAGE, INQUIRE ABOUT ITS GEOMETRY, AND PLOT VARIOUS VIEWS.

MUCH OF THE DISPLAY EDITING IS DONE IN TERMS OF "ATOM NAMES". THESE MUST BE PROVIDED ALONG WITH THE COORDINATES IN THE FIRST PHASE. THEY ARE MODIFIED IF SYMMETRY IS USED BY ADDING A SEVENTH AND EIGHT CHARACTER TO THE SIX ACCEPTED. SOME OF THE COMMANDS, E.G. "RNGE", ACCEPT THE FULL EIGHT CHARACTER NAME, WHILE OTHERS ALLOW ONLY THE SIX CHARACTER NAME OF THE ATOM. IN MATCHING NAMES AGAINST COMMANDS THE CHARACTER "*" IS USED TO MATCH ANY AND ALL CHARACTERS. THUS CA*1 WILL MATCH CA01, CA11, CAA1, ETC.

THE SEVENTH AND EIGHTH CHARACTERS ARE DETERMINED BY THE TRANSLATION USED AND THE SYMMETRY OPERATION USED. THE SYMMETRY OPERATIONS ARE GIVEN LETTERS FROM "A" THROUGH "X" IN THE ORDER IN WHICH THE USER PROVIDES THEM. THIS LETTER BECOMES THE EIGHTH CHARACTER OF THE ATOM NAME. THE SEVENTH CHARACTER IS "A" IF NO TRANSLATIONS ARE NEEDED. LETTERS ARE USED FURTHER DOWN THE ALPHABET AS MORE TRANSLATIONS ARE USED.

SOME PORTIONS OF THE PROGRAM INVOKE INTERACTIVE DIALOGS WITH THE USER. IN GENERAL, ONE MUST BE CAREFUL TO ANSWER THE QUESTIONS AS ASKED. WHEN NUMERIC INPUT IS REQUESTED, THE LAST NUMBER SHOULD BE TERMINATED BY A COMMA.

DATA INPUT BEFORE DISPLAY

DATA INPUT BEFORE THE DISPLAY CONSISTS OF CARD IMAGES READ FROM THE KEYBOARD OR ANY OTHER FILE. IN MOST CASES, THE ORDER OF THESE CARD IMAGES DOES NOT MATTER. THUS "CELL" MAY APPEAR EITHER BEFORE OR AFTER "ATOM" WITH THE SAME EFFECT. EACH CARD IMAGE CONTAINS A KEYWORD IN COLUMNS 1 THROUGH 4. THIS KEYWORD DETERMINES THE FORMAT OF THE REST OF THE CARD IMAGE. SPECIAL CARE MUST BE EXERCISED WITH "RNGE", "ATOM", "SYMT", AND "LATI", SINCE THEIR PARAMETERS DO NOT START IMMEDIATELY AFTER THE KEYWORD.

DMAX: SET MAXIMUM BONDING RADIUS (A4,F10.5)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "DMAX" 5-14 MAX BOND DIST	1.7 ANGSTROMS	VALUE ASSIGNED

NOTE -- 0.0 MEANS CHECK ATOM NAME VS. RADIUS LIST

DMIN: SET MINIMUM BONDING RADIUS (A4,F10.5)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "DMIN" 5-14 MIN BOND DIST	0.0 ANGSTROMS	VALUE ASSIGNED

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LINE: SET SOLID LINES FOR RNGE (A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "LINE"	USE LAST MODE SET	DRAW SOLID LINES

NOTE -- SOLID LINES ARE THE DEFAULT IF NO MODE WAS SET. THIS COMMAND NULLIFIES ANY PREVIOUS "DASH", "DOT ", OR "POIN" COMMAND.

DASH: SET DASH LINES FOR RNGE (A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "DASH"	USE LAST MODE SET	SET DASH MODE

NOTE -- THIS COMMAND NULLIFIES ANY PREVIOUS "LINE", "DOT ", OR "POIN" COMMAND.

DOT : SET DOT MODE FOR RNGE (A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "DOT "	USE LAST MODE SET	SET DOT MODE

NOTE -- THIS COMMAND NULLIFIES ANY PREVIOUS "LINE", "DASH", OR "POIN" COMMAND.

POIN: SET END POINT MODE FOR RNGE (A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 5 "POINT"	USE LAST MODE SET	SET END POINT MODE

NOTE -- THIS COMMAND NULLIFIES ANY PREVIOUS "LINE", "DASH", OR "DOT " COMMAND.

CELL: DEFINE UNIT CELL (A4,F17.5,2F8.5,3F9.6)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "CELL"	ACCEPT INPUT ATOMS	VALUES ASSIGNED
5-21 A	AS BEING IN CART-	
22-29 B	ESIAN COORDINATES	
30-37 C	(ORTHOGONAL AXES OF	
38-46 ALPHA	LENGTH 1 ANGSTROM)	
47-55 BETA		
56-64 GAMMA		

NOTE -- ANGLES AND COSINES MAY BE MIXED.

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RNGE: CONTROL BONDING OF ATOMS (A4,5(A8,2X),2F10.5)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "RNGE" 5- 8 LINE MODE 9-14 RESERVED 15-20 START RANGE 1 25-30 END RANGE 1 35-40 START RANGE 2 45-50 END RANGE 2 55-64 DMAX FOR RNGE 65-74 DMIN FOR RNGE	BOND ALL ATOMS WITH SEPARATION LESS THAN DMAX AND GREATER THAN DMIN	BOND ATOMS IN RANGE1 TO THOSE IN RANGE2 WHEN THE SEPARATION IS LESS THAN DMAX AND GREATER THAN DMIN

NOTE -- EACH RANGE IS SPECIFIED BY AN ATOM NAME TO MATCH. LINE MODE MAY BE THE LEFT JUSTIFIED CHARACTERS

LINE
DASH
DOT
POIN

OR BLANK TO USE LAST LINE, DASH, DOT, OR POIN COMMAND.

NOTE -- DMAX=0.0 MEANS TAKE VALUE FOR DMAX FROM LAST DMAX CARD. DMIN HAS A SIMILAR MEANING. IF NO NAMES APPEAR IN ONE RANGE, THEN BOTH RANGES ARE ASSUMED THE SAME. IF THE SECOND NAME OF A PAIR IS MISSING, IT IS SET EQUAL TO THE FIRST. IF ONLY THE FIRST NAME OF THE FIRST RANGE APPEARS, AND NO NAMES APPEAR FOR THE SECOND RANGE, THE NAMED ATOM IS BONDED TO ALL OTHERS. IF SYMMETRY CARDS ("SYMT") ARE USED, THE SIX CHARACTER ATOM NAMES MUST BE EXTENDED TWO CHARACTERS ON THE EXTREME RIGHT OF EACH FIELD. (I.E. IN COLUMNS 21-22, 31-32, 41-42, AND 51-52) ASTERISKS ARE RECOMMENDED, AS IN "CA101 **", UNLESS ONE IS TRYING FOR SPECIAL EFFECTS.

NOTE -- THE START OF A RANGE WILL BE THE FIRST MATCH OF THE NAME GIVEN, AND THE END OF A RANGE WILL BE THE LAST MATCH OF THE NAME GIVEN.

SIZE: SET PICTURE SIZE (A10,F10.5)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "SIZE" 5-14 MAX X-DIMENSION	12 INCHES IF GAIN IS AT MINIMUM	VALUES ASSIGNED

NOTE -- TOO LARGE A VALUE MAY SQUEEZE THE PICTURE AGAINST THE SIDES OF A LIMITING CUBE.

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ATOM: PROVIDE ATOM NAME AND COORDINATES (A4,3X,A6,3F8.5)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "ATOM" 8-13 ATOM NAME 14-21 X 22-29 Y 30-37 Z	NO ATOMS OR USE READ COMMAND (BELOW)	VALUES ASSIGNED

READ: READ COORDINATE FILE (A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "READ"	NO ATOMS OR USE ATOM COMMAND (ABOVE)	START SPECIAL SEGMENT FOR READING FROM UNIT 1 WITH INTERACTIVE CUES

NOTE -- SEE SECTION "INPUT TO READ COMMAND" BELOW.

NORM: SET INITIAL VIEW (A4,2(A6,4X))

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "NORM" 5-10 NAME 1ST ATOM 15-20 NAME 2ND ATOM	INITIAL VIEW DOWN Z-AXIS	INITIAL VIEW DOWN VECTOR CONNECTING 1ST ATOM TO 2ND ATOM

NOTE -- USES ONLY SIX CHARACTER ATOM NAMES. THIS MAY CAUSE SOME CONFUSION IF SYMMETRY IS USED. IN THAT CASE THE FIRST MATCH, USUALLY THE FIRST SYMMETRY ELEMENT, WILL BE USED.

PLAN: SET INITIAL VIEW (A4,3(A6,4X))

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "PLAN" 5-10 NAME 1ST ATOM 15-20 NAME 2ND ATOM 25-30 NAME 3RD ATOM	INITIAL VIEW DOWN Z-AXIS	INITIAL VIEW ONTO PLANE OF THE 3 ATOMS

NOTE -- USES ONLY SIX-CHARACTER ATOM NAMES.

SYMT: INPUT SYMMETRY OPERATION (A4,2X,74A1) OR (A4,2X,9F9.6)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 6 "SYMTRY"	NO MODIFICATION	APPLY THIS SYMOP
7-80 SYMMETRY OPERATION		

NOTE -- INPUT SYMMETRY INCLUDING X,Y,Z, THE IDENTITY TRANSFORM, EITHER AS IN THE INTERNATIONAL TABLES, OR AS ROWS OF A MATRIX, THEN THE VECTOR TRANSLATION. FOR EXAMPLE:

```
  SYMTRY -X,1/2+Y,-Z
```

OR

```
  SYMTRY -1.,0.,0.,0.,1.,0.,0.,0.,-1.,0.,0.5,0.,
```

SYMMETRY OPERATIONS RELATED BY A CENTER OF SYMMETRY AT THE ORIGIN NEED NOT BE INPUT IF THE "LATI" CARD, BELOW, IS USED TO PROVIDE SUCH SYMMETRY.

LATI: INPUT LATTICE (A4,4X,A1,2(,A1)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 6 "LATICE"	ACENTRIC PRIMITIVE	ADD LATTICE OPS
9 CENTRICITY CODE		
12 LATTICE TYPE		

NOTE -- THE CENTRICITY CODE MAY BE "A" FOR ACENTRIC, OR "C" FOR CENTROSYMMETRIC. THE LATTICE TYPE MAY BE "P", "A", "B", "C", "I", OR "F".

BOX : SET VOLUME TO BE FILLED (A4,6F10.4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "BOX "	IF SYMOPS GIVEN,	BOX FILLED USING
5-14 LOWER X LIMIT	SYMOPS APPLIED	CELL TRANSLATIONS
15-24 LOWER Y LIMIT	AS READ	
25-34 LOWER Z LIMIT	NO CELL TRANSLATIONS	
35-40 UPPER X LIMIT	APPLIED	
45-54 UPPER Y LIMIT		
55-64 UPPER Z LIMIT		

NOTE -- LIMITS ARE IN CELL EDGE FRACTIONS.

FILE: ASSIGN INPUT FILE (A4,6A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "FILE"	KB: (KEYBOARD)	FILES ASSIGNED TO 6
5-27 FILE IDENTIFIER		

NOTE -- THE COMMAND "FILE" MAY ALSO BE GIVEN AFTER THE DISPLAY IS UP TO CAUSE DISPLAY COMMANDS TO BE READ FROM A FILE.

END : END PHASE ONE INPUT (A4)

PARAMETERS	CARD ABSENT	CARD PRESENT
1- 4 "END "	EXPECT MORE INPUT	START COMPUTATION

CONTROL-D WILL BE ANSWERED BY
TYPE COMMAND FILE NAME
REPLY WITH AN ORDINARY DOS FILE IDENTIFIER (DEVICE:FILE[UIC]) AND THAT FILE WILL BE READ UNTIL "END " IS REACHED AT WHICH POINT INPUT IS TERMINATED AND PROCESSING BEGINS, OR AN EOF IS REACHED AND "TYPE COMMAND FILE NAME" APPEARS AGAIN. KB: IS A LEGAL REPLY.

INPUT TO READ COMMAND

WHEN THE READ COMMAND IS ENCOUNTERED, THE FOLLOWING SEQUENCE OF PROMPTS IS OUTPUT TO UNIT 5 (KB:)

```
TYPE ATOM FILE NAME
ATOM NAME


     0 NONE
     1 FIRST
     4 LAST

TYPE FORMAT BLANK=
SKIP N CARDS--END WITH COMMA
READ N ATOMS--END WITH COMMA

          (REPLY WITH NUMBER OF CARD TO READ/SKIP)
```

IF NO EOF WAS DETECTED THE NEXT LINES WILL BE:

```
TYPE--
     1 STOP READ      (RETURN TO COMMAND INPUT)
     2 SKIP           (GO SKIP SOME CARDS)
     3 READ           (GO READ SOME MORE ATOMS)
     4 NEW FORMAT     (GET A NEW FORMAT AND READ SOME MORE)
```

IF AN EOF IS DETECTED, THE REPLY IS "*" MEANING YOU ARE BACK IN COMMAND MODE CONTROL-D WILL GET ONE SAFELY OUT OF THE READ LOOP UNLESS ONE HAS TYPED "4" FOR NEW FORMAT OPTION.

THUS IN ORDER TO USE THE READ COMMAND TO INPUT ATOMIC COORDINATES, ONE MUST HAVE A FILE WITH NO MORE THAN ONE SET OF COORDINATES PER LINE, AND KNOW THE FORMAT. THE FIRST QUESTION ("FILE NAME") SHOULD BE ANSWERED WITH A STANDARD DOS FILE IDENTIFIER, E.G. "CR:". THE "ATOM NAME"

QUESTION REQUIRES A REPLY OF 0 IF THERE IS NO NAME FIELD, 1 IF THE NAME FIELD COMES BEFORE THE COORDINATES, AND 4 IF THE NAME FIELD COMES AFTER THE COORDINATES. THEN ONE MUST TYPE A FORMAT SPECIFICATION, INCLUDING OPEN AND CLOSE PARENTHESES. NOTE THAT INTERSPERSED TEMPERATURE FACTOR CARDS CAN BE SKIPPED BY INCLUDING A "/" IN THE FORMAT. ONE THEN PROVIDES A SKIP COUNT (OR CARRIAGE RETURN IF NONE ARE TO BE SKIPPED) FOLLOWED BY A READ COUNT.

DATA INPUT AFTER DISPLAY IS UP

ONCE THE COMMAND "END" HAS BEEN GIVEN, WHETHER FROM THE KEYBOARD OR FROM A FILE, PRJCTN COMPUTES THE CONNECTIVITY IMPLIED BY RNGE, DMAX, AND DMIN AFTER APPLYING THE SYMMETRY OPERATION. THE IMAGE IS SCALED AND CENTERED AND PUT ON THE DISPLAY SCREEN IN THE CHOSEN ORIENTATION. WHEN FIRST PUT UP, THE IMAGE IS STATIONARY. HITTING THE CARRIAGE RETURN (NEW LINE ON SOME MACHINES) WILL START THE IMAGE ROTATING ABOUT THE SCREEN VERTICAL AXIS. IT MAY BE STOPPED AGAIN BY HITTING THE SAME KEY. AT ANY TIME THE USER MAY TYPE A COMMAND. AFTER PROCESSING THE COMMAND, THE PICTURE WILL AGAIN BE STATIONARY.

THE COMMANDS "DIST", "ANGL", AND "TRSN" ALLOW TEMPORARY CHANGES IN THE IMAGE TO DISPLAY INTERESTING GEOMETRIC FEATURES VIA INTENSIFIED BONDS. COMMANDS SUCH AS "CLR" AND "PLOT" CAN REMOVE SUCH PORTIONS OF THE IMAGE. "NAME" IS SIMILARLY TEMPORARY. "BOND" AND "UNBD" SHOULD BE USED FOR MORE PERMANENT CHANGES.

DIST: BRIGHTEN BOND AND COMPUTE LENGTH (A4,2A6)

PARAMETERS	EFFECT OF COMMAND
1- 4 "DIST"	DRAW BOND BRIGHT AND PRINT LENGTH
5-10 1ST ATOM NAME	
11-16 2ND ATOM NAME	

NOTE -- IF NO NAME IS GIVEN, COMPUTE FOR ALL ATOMS. IF ONE NAME APPEARS, COMPUTE FOR THAT ATOM ONLY. IN THE CASE THAT DATA IS BEING COMPUTED FOR MORE THAN ONE COMBINATION OF ATOMS, A PROMPT WILL BE GIVEN FOR THE "PRINT FILE". THE ANSWER SHOULD BE LP:, FOR EXAMPLE, IF THE VOLUME OF OUTPUT IS EXPECTED TO BE LARGE. CARRIAGE RETURN GIVES LP: AS THE DEFAULT.

ANGL: BRIGHTEN ANGLE AND PRINT DEGREES (A4,3A6)

PARAMETERS	EFFECT OF COMMAND
1- 4 "ANGL"	DRAW ANGLE BRIGHT AND PRINT DEGREES
5-10 1ST ATOM NAME	
11-16 2ND ATOM NAME	
17-22 3RD ATOM NAME	

NOTE -- SEE NOTE FOR "DIST"

TRSN: - BRIGHTEN TORSION ANGLE AND PRINT DEGREES (A4,4A6)

PARAMETERS	EFFECT OF COMMAND
1- 4 "TRSN"	DRAW ANGLE BRIGHT AND PRINT DEGREES
5-10 1ST ATOM NAME	
11-16 2ND ATOM NAME	
17-22 3RD ATOM NAME	
23-28 4TH ATOM NAME	

NOTE -- SEE NOTE FOR "DIST"

CLR : CLEAR DISPLAY ITEMS ADDED (A4,I6)

PARAMETERS	EFFECT OF COMMAND
1- 4 "CLR "	TEMPORARY DISPLAY ITEMS CLEARED
5-10 # OF ITEMS	

NOTE -- SOME IMAGES CONSIST OF A LARGE NUMBER OF DISPLAY ITEMS. (I.E. A BRIGHT BOND WOULD CONSIST OF TWO DISPLAY ITEMS, A MOVE AND A DRAW)

GEOM: PRINT MOLECULAR GEOMETRY (A4)

PARAMETERS	EFFECT OF COMMAND
1- 4 "GEOM"	PRINT "DIST", "ANGL", "TRSN" OUTPUT

NOTE -- THIS COMMAND GIVES A COMPREHENSIVE CALCULATION OVER ALL BONDED ATOMS OF THE QUANTITIES OBTAINED SINGLY BY THE "DIST", "ANGL" AND "TRSN" COMMANDS. THE OUTPUT FROM "GEOM" SHOULD NORMALLY BE DIRECTED TO THE PRINTER BY ANSWERING THE FILE PROMPT WITH A CARRIAGE RETURN.

BOND/UNBD: CREATE OR REMOVE BOND (A4)

PARAMETERS	EFFECT OF COMMAND
1- 4 "BOND"/"UNBD"	ENTER DIALOG TO CREATE/REMOVE BONDS

NOTE -- THE COMMANDS "BOND" AND "UNBD" ARE IDENTICAL. THEY BOTH START A DIALOG WHICH ASKS "BOND OR UNBD", TO WHICH ONE MUST REPLY WITH EITHER OF THE TWO COMMANDS AGAIN. IF THE COMMAND IS "BOND" ONE WILL BE ASKED "LINE, DASH, DOT , OR POINT", TO WHICH ONE MUST REPLY WITH ONE OF THE FOUR LINE TYPES. FOR EITHER "BOND" OR "UNBD", ONE IS THEN ASKED FOR "FIRST ATOM NAME, DMAX, DMIN", TO WHICH ONE REPLIES WITH A FULL EIGHT CHARACTER ATOM NAME, FOLLOWED BY 2F10.4 NUMBERS. IF DMAX IS ZERO, IT IS TREATED AS INFINITY. THE SAME INPUT IS REQUIRED FOR THE QUESTION "SECOND ATOM NAME, DMAX, DMIN". ALL BONDS MEETING BOTH SETS OF DMAX/DMIN RESTRICTIONS ARE INSERTED IF "BOND" WAS REQUESTED. DMAX/DMIN ARE IGNORED FOR "UNBD". BLANK LINE INPUTS CAUSE THE DIALOG TO BACK UP ONE QUESTION, FINALLY RETURNING TO THE DISPLAY COMMANDS.

01-JUL-74 AUTHORS: L. MCCANDLISH, L. ANDREWS
01-JAN-76 REVISED: L. ANDREWS, H. BERNSTEIN

PRJCTN - 02/14/76

CIRC: DISPLAY CIRCLES AROUND ATOMS (A4,A6,F6.0)

PARAMETERS	EFFECT OF COMMAND
1- 4 "CIRC"	DISPLAY CIRCLES
5-10 ATOM NAME	
11-16 RADIUS	

NOTE -- THIS COMMAND HAS BEEN REMOVED IN SOME VERSIONS OF PRJCTN.

NAME: DISPLAY ATOM NAMES (A4,A8)

PARAMETERS	EFFECT OF COMMAND
1- 4 "NAME"	DISPLAY NAMES OF NAMED ATOMS
5-12 NAME TO MATCH	

NOTE -- IF SYMMETRY HAS BEEN USED, A FULL EIGHT CHARACTER ATOM NAME IS REQUIRED. IF "**" IS USED IN COLUMNS 11 AND 12, THE SAME ATOM IN ALL SYMMETRY ELEMENTS WILL ACQUIRE A NAME. IF, SAY, "AA" IS USED IN COLUMNS 11 AND 12, ONE THE REPRESENTATIVE IN THE FIRST SYMMETRY ELEMENT WILL BE NAMED.

ORTP: PRINT ORTEP ANGLES (A4)

PARAMETERS	EFFECT OF COMMAND
1- 4 "ORTP"	PRINT ANGLES IN ORDER 1, 3, 2

NOTE -- THE ORDER OF ANGLES GIVEN IS X, Z, Y. IN SOME VERSIONS OF PRJCTN, THE X AND Z ANGLES ARE THE NEGATIVES OF THE ONES REQUIRED BY ORTEP. THE ROTATIONS ARE ABOUT THE X, Y, Z AXES OF THE REFERENCE COORDINATE SYSTEM IN ORTEP.

CHNG - CHANGE VALUE OF CONTROL DIAL (A4,A6,F10.4)

PARAMETERS	EFFECT OF COMMAND
1- 4 "CHNG"	PROVIDES A USER VALUE FOR THE GIVEN FUNCTION
5-10 FUNCTION NAME	AND DISCONNECTS IT FROM THE DIAL
11-20 NEW VALUE	

NOTE -- EACH DIAL HAS A FUNCTION NAME ASSOCIATED WITH IT. TO ALLOW ROOM FOR JOY-STICK ENTRIES, THE CONTROL DIALS ARE NUMBERED FROM 4 THROUGH 13. "CHNG" ALLOWS ONE TO MIMIC DIALS FROM THE KEYBOARD. THE INITIAL FUNCTION NAMES AND ASSIGNMENTS ARE AS FOLLOWS.

FUNCTION NAME	FUNCTION ASSIGNMENT	
Y-AXIS	4 (DIAL 1)	
X-AXIS	5 (DIAL 2)	
Z-AXIS	6 (DIAL 3)	
IOFSET	7 (DIAL 4)	INTENSITY OFFSET
ISCALE	8 (DIAL 5)	INTENSITY SCALE
ROTRAT	9 (DIAL 6)	ROTATION RATE

THE VALUES TO BE GIVEN RANGE FROM -20.48 TO +20.48 TO MATCH EXTREME COUNTER-CLOCKWISE THROUGH EXTREME CLOCKWISE ROTATION. THIS IS JUST A RANGE OF PURE NUMBERS WITH NO SPECIFIC MEANING.

RENM: RENAME CONTROL DIAL FUNCTION (A4,A6,A6)

PARAMETERS	EFFECT OF COMMAND
1- 4 "RENM"	CHANGE OLD FUNCTION NAME TO NEW
6-10 OLD NAME	
11-16 NEW NAME	

NOTE -- SEE NOTE FOR CHNG.

ASGN: ASSIGN CONTROL DIAL TO FUNCTION (A4,A6,I5)

PARAMETERS	EFFECT OF COMMAND
1- 4 "ASGN"	CHANGE CONTROL DIAL ASSIGNED TO FUNCTION
5-10 FUNCTION NAME	GIVING POSITIVE NUMBER (4-13) FOR DIAL (1-10)
11-15 NEW NUMBER	OR NEGATIVE FOR INCREMENTAL MODE, 0 FOR NONE

NOTE -- SEE NOTE FOR CHNG

VALU: PRINT CURRENT ASSIGNMENTS AND VALUES (A4)

PARAMETERS	EFFECT OF COMMAND
1- 4 "VALU"	PRINT LIST OF CURRENT VALUES AND ASSIGNMENTS

PLOT: PLOT CURRENT DISPLAY (A4)

PARAMETERS	EFFECT OF COMMAND
1- 4 "PLOT"	ENTER DIALOG TO CREATE PLOT IMAGE

NOTE -- THE DIALOG WILL ASK FOR THE "PLOT FILE" FIRST. A CARRIAGE RETURN WILL CAUSE USE OF VP:, THE VERSATEC PLOTTER. OTHER DEVICES CAN BE ASSIGNED TO SAVE THE PLOT IMAGE. BE WARNED THE IMAGE IS TOO LARGE TO BE STORED AS A LINKED FILE ON DISC. THE NEXT QUESTION ASKS FOR CENTIMETERS PER ANGSTROM, NUMBER OF IMAGES, AND Z-OFFSET. THE ANSWER SHOULD BE THREE NUMBERS, SEPARATED BY COMMAS, OR JUST A CARRIAGE RETURN.

CENTIMETERS PER ANGSTROM IS A FLOATING POINT NUMBER CONTROLLING THE PICTURE SIZE. IF THE PICTURE WILL NOT FIT ON ONE PAGE FOR THE SIZE GIVEN, IT IS BROKEN INTO MULTIPLE PAGES. IF THE SIZE GIVEN IS ZERO, THE PICTURE WILL BE SCALED TO FIT ONE PAGE. NIMAGE IS THE NUMBER OF 6 DEGREE ROTATIONS TO PLOT. THE FIRST PLOT WILL AGREE WITH THE LAST SCREEN IMAGE. THE NEXT IMAGE IS ROTATED SIX DEGREES AROUND THE Y-AXIS IN THE POSITIVE SENSE. IF NIMAGE IS ZERO, ONE IMAGE WILL BE PLOTTED. THE Z OFFSET CONTROLS THE USE OF DOT SKIPPING TO SIMULATE DEPTH CUEING. A LARGE NUMBER (999.) WILL SUPPRESS ALL SHADING.

NOTE ON NUMERIC INPUT

WHEN USED IN THE STANDARD CRYSNET RELEASE SYSTEM, PRJCTN ALLOWS NUMERIC FIELDS TO BE TERMINATED BY COMMAS. THE COMMA IS PART OF THE FIELD, NOT A SPECIAL COMMAND. THUS, IF A FORMAT SPECIFIES F10.4 INPUT, A FULL TEN DIGITS MAY BE TYPED, OR FEWER DIGITS MAY BE TYPED, AND THE FIELD TERMINATED BY A COMMA. HOWEVER, AN ERROR MAY RESULT IF A FULL TEN DIGITS ARE TYPED AND A COMMA IS ADDED AS WELL, SINCE THE COMMA WILL THEN BE IN THE NEXT FIELD, AND TERMINATE THAT ONE INSTEAD OF THE ONE INTENDED. A COMMA WILL ALSO TERMINATE AN X-FIELD, BUT NOT AN A-FIELD, SO SOME FLEXIBILITY IS ALLOWED ON "RNGE" COMMANDS. HOWEVER, ATOM NAMES (WHICH ARE ALPHABETIC INFORMATION) MUST BE SPELLED OUT WITH ALL TRAILING BLANKS.

I N D E X

COMMANDS
ANGL - BRIGHTEN ANGLE AND PRINT DEGREES PRJCTN-9
ASGN - ASSIGN CONTROL DIAL TO FUNCTION PRJCTN-12
ATOM - PROVIDE ATOM NAME AND COORDINATES PRJCTN-6
BOND - CREATE OR REMOVE BOND PRJCTN-10
BOX - SET VOLUME TO BE FILLED PRJCTN-7
CELL - DEFINE UNIT CELL PRJCTN-4
CHNG - CHANGE VALUE OF CONTROL DIAL PRJCTN-11
CIRC - DISPLAY CIRCLES AROUND ATOMS PRJCTN-11
CLR - CLEAR DISPLAY ITEMS PRJCTN-10
DASH - SET DASH LINES FOR RNGE PRJCTN-4
DIST - BRIGHTEN BOND AND COMPUTE LENGTH PRJCTN-9
DMAX - SET MAXIMUM BONDING RADIUS PRJCTN-3
DMIN - SET MINIMUM BONDING RADIUS PRJCTN-3
DOT - SET DOT MODE FOR RNGE PRJCTN-4
END - END PHASE ONE INPUT PRJCTN-8
FILE - ASSIGN INPUT FILE PRJCTN-7
GEOM - PRINT MOLECULAR GEOMETRY PRJCTN-10
LATI - INPUT LATTICE PRJCTN-7
LINE - SET SOLID LINES FOR RNGE PRJCTN-4
NAME - DISPLAY ATOM NAMES PRJCTN-11
NORM - SET INITIAL VIEW PRJCTN-6
ORTP - PRINT ORTEP ANGLES PRJCTN-11
PLAN - SET INITIAL VIEW PRJCTN-6
PLOT - PLOT CURRENT DISPLAY PRJCTN-12
POIN - SET END POINT MODE FOR RNGE PRJCTN-4
READ - READ COORDINATE FILE PRJCTN-6
RENM - RENAME CONTROL DIAL FUNCTION PRJCTN-12
RNGE - CONTROL BONDING OF ATOMS PRJCTN-5
SIZE - SET PICTURE SIZE PRJCTN-5
SYMT - INPUT SYMMETRY OPERATION PRJCTN-7
TRSN - BRIGHTEN TORSION ANGLE AND PRINT DEGREES PRJCTN-10
UNBD - CREATE OR REMOVE BOND PRJCTN-10
VALU - PRINT CURRENT ASSIGNMENTS AND VALUES PRJCTN-12
COMMAS TO TERMINATE FIELDS PRJCTN-13
DATA INPUT AFTER DISPLAY IS UP PRJCTN-9
DATA INPUT BEFORE DISPLAY PRJCTN-3
DIAL FUNCTIONS PRJCTN-2
INTRODUCTION PRJCTN-2
LIMITATIONS PRJCTN-1
LOGICAL UNITS PRJCTN-2
NUMBERIC INPUT PRJCTN-13
READ COMMAND INPUT PRJCTN-8
STEREO DISPLAY PRJCTN-2
SWITCH SETTINGS PRJCTN-1
SYMMETRY PRJCTN-1

PROGRAM NAME	RSTD
PURPOSE	checks standard reflections from data collection
LIMITATIONS	
SWITCH SETTINGS	
LOGICAL UNITS	6 KB for input information
FILE ASSIGNMENTS	none must log in as [1,11] magnetic tape with data must be mounted

SANDA

```
                                                                    ↑S
.KI
$  TO COMPILE USE SANDA,LP:<SANDA.SRC/ON/CK                    ↑U
RUN LINK
LINK V11A01
#SANDA<SANDA/CC,FTNLIB/L/U/E

TRANSFER ADDRESS: 024164
LOW LIMIT: 024164
HIGH LIMIT: 077460

LINK V11A01
#↑C
.KI
$AS CR:,4
$AS LP:,5
$AS DK:JUNK,3
$ NOTE*******ON HELEN'S SYSTEM THAT SHOULD BE KB: NOT LP:   ↑U
NOTE ESPECIALLY THAT JUNK NEEDS TO BE DELETED BEFORE YOU RUN AGAIN   ↑U
RUN SANDA

I350 000000

$I AM GOING TO PUT A COPY OF R\R\FRANCIS7S TEST DECK ON LP:    ↑U
LP:↑U
RUN PIP
PIP-11  V7A01
#JUNK/DE

#R\R\LP:<CR:

#↑C
.KI
$FI
TIME:-15:39:13

DOS V08-02

$
```

```
      C     INTRAMOLECULAR AND INTERMOLECULAR DISTANCES
      C                 CRYSTALLOGRAPHY LABORATORY, UNIV. OF PITTSBURGH
      C                           R.SHIONO AND SHIRLEY S.C.CHU
      C                              MAY 1964 AND FEBRUARY 1965
      C                                     R.SHIONO
      C                          APRIL 1968, FEB. 1969, NOV. 1969.
      C          SCRATCH TAPE ON UNIT 3
      C     IS1 =0 FOR LINUS ATOM FORMAT (ALSO UCLALS), 1 FOR XRAY-63,
      C         2 FOR ORFLS
      C     IS2=2 FOR DECIMAL FRACTIONS, 1 FOR GRID COORDINATES
      C
      C     FRANCES C. BERNSTEIN  BNL  9/73
      C     FIX UP FORMATS FOR FOCUS 58 CHAR LIMIT
      C
0001        COMMON A1,A2,A3,B1,B2,B3,TITLE
0002        COMMON  U,V,W,C1,C2,C3,NT
0003        DIMENSION C1(12),I1(12),J1(12),C2(12),I2(12),J2(12),C3(12),
           2  I3(12),J3(12) ,U(40),V(40),W(40),P(7),NP(3,40),AIDAB(40)
0004        DIMENSION  TITLE(20),MSY(7),ORCD(3)
0005        DIMENSION TST(4,60),KST(3,60),NT(50)
0006        DATA MSY / 2H-Z,2H-Y,2H-X,2H  ,2H+X,2H+Y,2H+Z /
0007        REWIND 3
      C     CONSTANTS FOR ALPHABETIC +X,-X,+Y      ETC.
0008        READ 71, (TITLE(K),K=1,20)
0009        PRINT 70,TITLE
      C     READ THE CELL CONSTANT CARD
0010        READ 73, A1,A2,A3,B1,B2,B3
0011        JTRN=27
0012        READ 78, N,M,NCARD, DMAX,DMIN,IAGL,DANG,ITRN,ISOR,TR,TS,TT,IS1,IS2
0013        IS1 = IS1 + 1
0014        IF (DMAX .EQ. 0.0) DMAX = 1.7
0015        IF (TR .EQ. 0.0) TR = 1.0
0016        IF (TS .EQ. 0.0) TS = 1.0
0017        IF (TT .EQ. 0.0) TT = 1.0
0018        QR = 1./TR
0019        QS = 1./TS
0020        QT = 1./TT
0021        IF  ( ITRN )  87,  87,  86
0022     86 JTRN=1
0023     87 IAGL=IAGL+1
0024        NCARD=NCARD+1
      C     READ SYMMETRY CARDS
0025        READ 75, (C1(K),I1(K),J1(K),C2(K),I2(K),J2(K),C3(K),I3(K),J3(K),
           1K=1,M)
0026        PRINT 79
0027        DO  61  L=1,M
0028        K1=I1(L)+4
0029        K2=J1(L)+4
0030        K3=I2(L)+4
0031        K4=J2(L)+4
0032        K5=I3(L)+4
0033        K6=J3(L)+4
0034     61 PRINT 80,L,C1(L),MSY(K1),MSY(K2),C2(L),MSY(K3),MSY(K4),C3(L),
           1MSY(K5),MSY(K6)
0035        IF  (DANG)  88,  88,  208
```

```
0036      88    DANG=DMAX
0037      208 GO TO(201,97,301),IS1
0038      301 DO 302 K=1,N
0039          READ 303,U(K),V(K),W(K),AIDAB(K)
0040          GO TO (302,305),NCARD
0041      305 READ 303
0042      302 CONTINUE
0043          GO TO 204
0044      201 DO 202 K = 1,N
0045          READ 203, AIDAB(K),U(K), V(K), W(K)
0046          GO TO (202,205), NCARD
0047      205 READ 203
0048      202 CONTINUE
0049          GO TO 204
0050      97  DO  146  K=1,N
0051          READ 74,AIDAB(K),U(K),V(K),W(K)
0052          GO TO(151,152),IS2
0053      151 U(K) = U(K)*QR
0054          V(K) = V(K)*QS
0055          W(K) = W(K)*QT
0056      152 GO TO ( 146, 147), NCARD
0057      147 READ 74
0058      146 CONTINUE
0059      204 PRINT 8, DMAX, DMIN
0060          PRINT 93,A1,A2,A3,B1,B2,B3
0061          PRINT 190
0062          DO 191 K = 1,N
0063          PRINT 192,K,AIDAB(K),U(K), V(K), W(K)
0064      191 CONTINUE
0065          PRINT 72
        C     ADJUST THE COORDINATES TO WITHIN ONE HALF
0066          DO  39  L=1,N
0067          NP(1,L)=0
0068          NP(2,L)=0
0069          NP(3,L)=0
0070          IF ( ITRN )  180,  180,  39
0071      180 IF ( ABS(U(L))-0.5 )  64,  64,  63
0072      63  NP(1,L)=SIGN(1.0,U(L))
0073          IF   (U(L))   65,  64,  66
0074      65  U(L)=U(L)+1.
0075          GO TO 64
0076      66  U(L)=U(L)-1.
0077      64  IF  ( ABS(V(L) ) -0.5 )  67,  67,  68
0078      68  NP(2,L)=SIGN(1.0,V(L))
0079          IF   (V(L))   69,  67,  51
0080      69  V(L)=V(L)+1.
0081          GO TO 67
0082      51  V(L)=V(L)-1.
0083      67  IF  ( ABS(W(L) ) -0.5 )  39,  39,  52
0084      52  NP(3,L)=SIGN(1.0,W(L))
0085          IF   (W(L))   53,  39,  54
0086      53  W(L)=W(L)+1.
0087          GO TO 39
0088      54  W(L)=W(L)-1.
0089      39  CONTINUE
0090          DMIN=DMIN*DMIN
```

```
0091            MTWO=DMAX+DMAX
0092            DMA=DMTWO
0093            DMB=DMTWO
0094            DMC=DMTWO
0095            JA=1
0096            JB=1
0097            JC=1
0098            DMSQ=DMAX*DMAX
0099            IF  (B1)  43, 40, 43
0100       40   JA=2
0101            IF  (B2)  48, 41, 48
0102       41   JB=2
0103            DMC=DMAX
0104            IF  (B3)  9, 42, 9
0105       42   DMB=DMAX
0106            DMA=DMAX
0107            JA=3
0108            GO TO 9
0109       43   IF  (B2)  44, 46, 44
0110       44   IF  (B3)  9, 50, 9
0111       45   JB=2
0112            IF  (B3)  9, 47, 9
0113       47   DMA=DMAX
0114            GO TO 50
0115       48   IF  (B3)  9, 49, 9
0116       49   DMB=DMAX
0117       50   JC=2
          C     LOOP FOR THE STARTING ATOM  1-N
0118        9   DO  60  L=1,N
0119            KDIS=0
          C     FOR THE ENDING ATOMS   1-N
0120            DO  62  K=1,N
0121            P(4)=0.0
0122            P(5)=U(K)
0123            P(3)=-P(5)
0124            P(6)=V(K)
0125            P(2)=-P(6)
0126            P(7)=W(K)
0127            P(1)=-P(7)
          C     GO THROUGH ALL SYMMETRY RELATIONS   1-M
0128            DO 62 I=1,M
0129            M1=I1(I)+4
0130            N1=J1(I)+4
0131            M2=I2(I)+4
0132            N2=J2(I)+4
0133            M3=I3(I)+4
0134            N3=J3(I)+4
0135            NPX=0
0136            NPY=0
0137            NPZ=0
0138            IJ=IABS(I1(I))
0139            IF  ( IJ )  111,  111,  110
0140      110   NPX=NPX+NP(IJ,K)*ISIGN(1,I1(I))
0141      111   IJ=IABS(J1(I))
0142            IF  ( IJ )  113,  113,  112
0143      112   NPX=NPX+NP(IJ,K)*ISIGN(1,J1(I))
```

```
0144      113  IJ=IABS(I2(I))
0145           IF  (  IJ )  115,  115,  114
0146      114  NPY=NPY+NP(IJ,K)*ISIGN(1,I2(I))
0147      115  IJ=IABS(J2(I))
0148           IF  ( IJ )  117,  117,  116
0149      116  NPY=NPY+NP(IJ,K)*ISIGN(1,J2(I))
0150      117  IJ=IABS(I3(I))
0151           IF  ( IJ )  119,  119,  118
0152      118  NPZ=NPZ+NP(IJ,K)*ISIGN(1,I3(I))
0153      119  IJ=IABS(J3(I))
0154           IF  ( IJ )  121,  121,  120
0155      120  NPZ=NPZ+NP(IJ,K)*ISIGN(1,J3(I))
0156      121  X=C1(I)+P(M1)+P(N1)
0157           Y=C2(I)+P(M2)+P(N2)
0158           Z=C3(I)+P(M3)+P(N3)
0159           DO  62  J=1,JTRN
0160           GO TO (11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30
              1,31,32,33,34,35,36,37),J
0161      11   E=X
0162           R=Y
0163           G=Z
0164           NTRR=555
0165           GO TO 45
0166      12   E=1.+X
0167           NTRR=655
0168           GO TO 45
0169      13   E=X
0170           R=1.+Y
0171           NTRR=565
0172           GO TO 45
0173      14   R=Y
0174           G=1.+Z
0175           NTRR=556
0176           GO TO 45
0177      15   E=-1.+X
0178           G=Z
0179           NTRR=455
0180           GO TO 45
0181      16   E=X
0182           R=-1.+Y
0183           NTRR=545
0184           GO TO 45
0185      17   R=Y
0186           G=-1.+Z
0187           NTRR=554
0188           GO TO 45
0189      18   E=1.+X
0190           R=1.+Y
0191           G=Z
0192           NTRR=665
0193           GO TO 45
0194      19   E=X
0195           G=1.+Z
0196           NTRR=566
0197           GO TO 45
0198      20   E=1.+X
```

```
0199            Y
0200          NTRR=656
0201          GO TO 45
0202     21   E=-1.+X
0203          R=-1.+Y
0204          G=Z
0205          NTRR=445
0206          GO TO 45
0207     22   E=X
0208          G=-1.+Z
0209          NTRR=544
0210          GO TO 45
0211     23   E=-1.+X
0212          R=Y
0213          NTRR=454
0214          GO TO 45
0215     24   E=1.+X
0216          R=-1.+Y
0217          G=Z
0218          NTRR=645
0219          GO TO 45
0220     25   E=-1.+X
0221          R=1.+Y
0222          NTRR=465
0223          GO TO 45
0224     26   E=X
0225          G=-1.+Z
0226          NTRR=564
0227          GO TO 45
0228     27   R=-1.+Y
0229          G=1.+Z
0230          NTRR=546
0231          GO TO 45
0232     28   E=-1.+X
0233          R=Y
0234          NTRR=456
0235          GO TO 45
0236     29   E=1.+X
0237          G=-1.+Z
0238          NTRR=654
0239          GO TO 45
0240     30   R=1.+Y
0241          G=1.+Z
0242          NTRR=666
0243          GO TO 45
0244     31   G=-1.+Z
0245          NTRR=664
0246          GO TO 45
0247     32   R=-1.+Y
0248          G=1.+Z
0249          NTRR=646
0250          GO TO 45
0251     33   E=-1.+X
0252          R=1.+Y
0253          NTRR=466
0254          GO TO 45
```

```
0255      34   E=1.+X
0256           R=-1.+Y
0257           G=-1.+Z
0258           NTRR=644
0259           GO TO 45
0260      35   E=-1.+X
0261           R=1.+Y
0262           NTRR=464
0263           GO TO 45
0264      36   R=-1.+Y
0265           G=1.+Z
0266           NTRR=446
0267           GO TO 45
0268      37   G=-1.+Z
0269           NTRR=444
0270      45   D4=0.
0271           D1=A1*(U(L)-E)
0272           IF  (D1-DMA)  55, 55, 62
0273      55   D2=A2*(V(L)-R)
0274           IF  (D2-DMB)  56, 56, 62
0275      56   D3=A3*(W(L)-G)
0276           IF  (D3-DMC)  57, 57, 62
0277      57   GO TO (58, 59, 84), JA
0278      58   D4=D4+D2*D3*B1
0279      59   GO TO ( 81, 82), JB
0280      81   D4=D4+D3*D1*B2
0281      82   GO TO ( 83, 84), JC
0282      83   D4=D4+D1*D2*B3
0283      84   DIST=D1*D1+D2*D2+D3*D3+D4+D4
0284           IF  (DIST-DMSQ)  85, 85, 62
0285      85   IF  ( DIST )  62,  122, 140
0286     140   IF  ( DIST-DMIN )  62,  122,  122
0287     122   DIST=SQRT(DIST)
0288           IF  ( NP(1,L) ) 130,  132,  131
0289     130   E=E-1.0
0290           GO TO 132
0291     131   E=E+1.0
0292     132   IF  ( NP(2,L) )  133,  135,  134
0293     133   R=R-1.0
0294           GO TO 135
0295     134   R=R+1.0
0296     135   IF  ( NP(3,L) )  136,  138,  137
0297     136   G=G-1.0
0298           GO TO 138
0299     137   G=G+1.0
0300     138   NTRR=NTRR+(NP(1,L)-NPX)*100+(NP(2,L)-NPY)*10+NP(3,L)-NPZ
0301           GO TO ( 148, 148, 141 ), IAGL
         C     IF STORAGE SPACE IS TIGHT, THIS SORTING PART MAY BE OMMITTED OR
         C         LINKED
         C     OMIT THE DISTANCE TO ITSELF
0302     148   IF ( DIST )  173,  173,  174
0303     173   IF ( NTRR-555 )  174,  175,  174
0304     175   IF ( L-K )  174,  176,  174
0305     176   IF ( I-1 )  174,  141,  174
0306     174   IF ( ISOR )  142,  142,  149
0307     142   MTX=C1(I)*100.
```

```
0308            MY=C2(I)*100.
0309           MTZ=C3(I)*100.
0310           PRINT 77,L,K,DIST,E,R,G,I,NTRR
       C       PRINT 77,L,K,DIST,E,R,G,MTX,MSY(M1),MSY(N1),MTY,MSY(M2),MSY(N2),
       C      1MTZ,MSY(M3),MSY(N3),I,NTRR
0311           GE = E*TR
0312           GR = R*TS
0313           GG = G*TT
0314           GO TO 141
       C       PREPARE FOR SORTING THE DISTANCES
0315      149  KDIS=KDIS+1
0316           KST(1,KDIS)=K
0317           KST(2,KDIS)=I
0318           KST(3,KDIS)=NTRR
0319           TST(1,KDIS)=DIST
0320           TST(2,KDIS)=E
0321           TST(3,KDIS)=R
0322           TST(4,KDIS)=G
0323      141  GO TO ( 62, 92, 92 ), IAGL
0324       92  IF  (DIST-DANG)  98,  98,  62
0325       98  WRITE (3)    L,K,DIST,E,R,G,I,NTRR
0326       62  CONTINUE
0327           IF ( ISOR )  60,  60,  160
       C       START SORTING DATA
0328      160  NDATA=KDIS
0329           IF  ( NDATA )  60,  60,  161
0330      161  M1=NDATA
0331      163  M1=M1/2
0332           IF ( M1 )  164,  170,  164
0333      164  M2=NDATA-M1
0334           M3=1
0335      165  M4=M3
0336      166  M5=M4+M1
0337           IF ( TST(1,M4)-TST(1,M5) )  168,  168,  167
0338      167  DO  169  IJ=1,4
0339           AHOLD=TST(IJ,M4)
0340           TST(IJ,M4)=TST(IJ,M5)
0341      169  TST(IJ,M5)=AHOLD
0342           DO  172  IJ=1,3
0343           IHOLD=KST(IJ,M4)
0344           KST(IJ,M4)=KST(IJ,M5)
0345      172  KST(IJ,M5)=IHOLD
0346           M4=M4-M1
0347           IF ( M4-1 )  168,  166,  166
0348      168  M3=M3+1
0349           IF ( M3-M2 )  165,  165,  163
       C       END OF SORTING
0350      170  DO  171  IJ=1,NDATA
0351           I=KST(2,IJ)
0352           MTX=C1(I)*100.0
0353           MTY=C2(I)*100.0
0354           MTZ=C3(I)*100.0
0355           M1=I1(I)+4
0356           N1=J1(I)+4
0357           M2=I2(I)+4
0358           N2=J2(I)+4
```

```
0359          M3=I3(I)+4
0360          N3=J3(I)+4
0361      171 PRINT 77,L,KST(1,IJ),(TST(IK,IJ),IK=1,4),I,KST(3,IJ)
        C 171 PRINT 77,L,KST(1,IJ),(TST(IK,IJ),IK=1,4),MTX,MSY(M1),MSY(N1),MTY,
        C    1MSY(M2),MSY(N2),MTZ,MSY(M3),MSY(N3),I,KST(3,IJ)
0362       60 CONTINUE
0363          GO TO ( 38, 99, 99), IAGL
0364       99 L=0
0365          K=0
0366          DIST=0.
0367          WRITE (3)    L,K,DIST,E,R,G,I,NTRR
        C     GO TO CALCULATE ANGLES
        C              THIS SUBROUTINE MAY BE SEPARATED IF NOT ENOUGH STORAGE
0368          CALL ANGLE
0369       38 PRINT 94
0370          STOP
0371        8 FORMAT(6X,5HDMAX=,F6.2,2X,5HDMIN=,F6.2)
0372       70 FORMAT(1H1,20A4)
0373       71 FORMAT ( 20A4 )
0374      203 FORMAT (A4, 2X, 21X, 3F9.6)
0375      303 FORMAT(3F10.5,40X,A4)
        C  72 FORMAT (3X,@ATOMS@,3X,@DISTANCE@,6X,@X@,8X,@Y@,8X,@Z@,10X,@SYMMETR
        C    1Y@,12X,@TRLN,@,2X,/)
0376       72 FORMAT (3X,5HATOMS,3X,9HDISTANCES,6X,1HX,8X,1HY,8X,1HZ,5X,3HSYM,2X
            2 ,4HTRLN)
0377       73 FORMAT ( 3F7.3, 3F7.4  )
0378       74 FORMAT (7X,A4,2X,3F8.4)
0379       75 FORMAT  ( F11.6, 2I2,F11.6,2I2,F11.6, 2I2  )
0380       77 FORMAT(1XI3,I4,F10.4,2X,3F9.5,3X,I3,2X,I3)
        C  77 FORMAT(1XI3,I4,F10.4,2X,3F9.5,1X,I3,2A2,I3,2A2,I3,2A2,1X,I3,2X,I3)
0381       78 FORMAT(3I4,2F6.2,I4,F6.2,2I4,3F4.0,2I4)
0382       79 FORMAT(3X,3HNO., 4X,8HSYMMETRY )
0383       80 FORMAT(1X,I4,3(F7.3,2X,2A3))
0384       93 FORMAT ( 1H ,4X,2HA=,F8.3,4H, B=,F8.3,4H, C=,F8.3,/7H, COSA=,F7.4,
            1         7H, COSB=,F7.4,7H, COSC=,F7.4  )
0385       94 FORMAT(5H END.)
0386      190 FORMAT (4X,11HINPUT ATOMS,5X,1HX,8X,1HY,8X,1HZ)
0387      192 FORMAT(1X,I4,2X,A4,2X,3F10.5)
0388      193 FORMAT (1H1)
0389      711 FORMAT(1H1,20A4,/)
0390          END
```

```
ROUTINES CALLED:
ABS    , SIGN   , IABS   , ISIGN , SQRT   , ANGLE

SWITCHES = /ON,/CK

BLOCK        LENGTH
MAIN.    5297    (024542)*
.$$$$.   414     (001474)

**COMPILER ----- CORE**
   PHASE        USED  FREE
DECLARATIVES 00705 04902
EXECUTABLES  01727 03880
ASSEMBLY     03205 05319
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        C       ALCULATION OF ANGLES FROM DISTANCE PROGRAM RESULTS
        C           CALCULATES ALL ANGLES, REJECTS REDUNDANT POSITIONS
        C                                   BY R.SHIONO   APRIL 1963
        C                            MODIFIED   MARCH 1965
        C                   REVISED FOR NEW FORMAT       DEC. 1966
        C
0001            SUBROUTINE ANGLE
0002            COMMON A,B,C,COSA,COSB,COSC,TITLE
        C       THESE VALUES ARE IN COMMON TO SAVE STORAGE SPACE
0003            COMMON X,Y,Z,D,M,NS,NT
0004            DIMENSION M(12),X(40),Y(40),Z(40),D(12),NS(12),NT(50)
0005            DIMENSION  TITLE(20)
0006            REWIND 3
0007            KLP=1H(
0008            KRP=1H)
0009            PRINT 8,KLP,KRP,KLP,KRP
0010            READ (3)    N1,M(1),D(1),X(1),Y(1),Z(1),NS(1),NT(1)
0011       41   N0=N1
0012            I=1
0013            GO TO 30
0014       17   I=I+1
0015         38 READ (3)    N1,M(I),D(I),X(I),Y(I),Z(I),NS(I),NT(I)
0016       39   IF  (N1-N0)   11,  30,  11
0017       30   IF  (N1-M(I))  10, 31,  10
0018       31   IF  (NS(I)-1)  10, 32, 10
        C32     IF  ( NT(I)-555 )  10,  46,  10
        C       CENTRAL ATOM WITH ZERO DISTANCE
        C       GO TO 38
0019       32   IF  ( NT(I)-555 )  10,  38,  10
0020       10   IF  ( D(I) )  38,  38,  23
0021       23   IF  ( I-1 )  17,  17,  34
0022       34   II=I-1
0023            DO  35  N=1,II
0024            IF  (X(I)-X(N))  35, 36, 35
0025       36   IF  (Y(I)-Y(N))  35, 37, 35
0026       37   IF  (Z(I)-Z(N))  35, 38, 35
0027       35   CONTINUE
0028            GO TO 17
0029       11   K=I-1
0030            IF  (K-2)  18, 12, 12
0031       12   K1=K-1
0032            DO  43  J=1,K1
0033            K2=J+1
0034            DO  14  L=K2,K
0035            A1=(X(J)-X(L))*A
0036            B1=(Y(J)-Y(L))*B
0037            C1=(Z(J)-Z(L))*C
0038            IF  (A1)  27, 25, 27
0039       25   IF  (B1)  27, 26, 27
0040       26   IF  (C1)  27, 14, 27
0041       27   DS=A1*A1+B1*B1+C1*C1+2.*(A1*B1*COSC+B1*C1*COSA+C1*A1*COSB)
0042            AG=.5*(-DS+D(J)*D(J)+D(L)*D(L))/(D(J)*D(L))
0043            IF  (AG)  15,16,15
0044       15   AGSQ=AG*AG
0045            IF  (1.-AGSQ)  28,  28,  29
```

```
0046      29   AGL=ATAN(SQRT(1.0-AGSQ)/AG)*57.29578
0047           IF  (AGL)  13, 42, 22
0048      13   AGL=180.+AGL
0049           GO TO 22
0050      28   AGL=0.
0051      42   DS=SQRT(DS)+0.001
0052           IF  (D(J)+D(L)-DS)  13, 13, 22
0053      16   AGL=90.
0054        22 PRINT 3,M(J),KLP,NS(J),NT(J),KRP,N0,M(L),KLP,NS(L),NT(L),KRP,D(J),
          1D(L),AGL
0055      14   CONTINUE
0056      43   CONTINUE
0057      18   IF  (N1)  19, 19, 40
0058      40   M(I)=M(I)
0059           X(I)=X(I)
0060           Y(I)=Y(I)
0061           Z(I)=Z(I)
0062           D(I)=D(I)
0063           NS(I)=NS(I)
0064           NT(I)=NT(I)
0065           GO TO 41
0066      19   RETURN
0067         3 FORMAT(1X,I3,1X,A1,I3,I4,1X,A1,2I4,1X,A1,I3,I4,1X,A1,2F7.3,F7.2)
0068         8 FORMAT(1X,6HATOM B,11X,1HA,2X,6HATOM C, 9X,1HD,A1,2HBA,A1,2X,1HD,
          1A1,2HAC,A1,2X,5HANGLE)
0069           END
```

```
ROUTINES CALLED:
ATAN  , SQRT

SWITCHES = /ON,/CK

BLOCK        LENGTH
ANGLE    1039    (004036)*
.$$$$.   390     (001414)

**COMPILER ----- CORE**
   PHASE        USED  FREE
DECLARATIVES  00545 05062
EXECUTABLES   00847 04760
ASSEMBLY      01657 06867
```

TEST OF SP

NO.	SYMMETRY					
1	0.000	+X	0.000	+Y	0.000	+Z
2	0.000	-X	0.500	+Y	0.000	-Z

DMAX= 2.00 DMIN= 0.00

A= 7.407, B= 5.301, C= 14.614

COSA= 0.0000, COSB=-0.1500, COSC= 0.0000

INPUT ATOMS		X	Y	Z
1	CL	0.11339	0.25000	0.12018
2	O1	0.60052	0.40669	0.07084
3	O2	0.41729	0.63305	0.14558
4	C	0.56695	0.59213	0.11089
5	CA	0.69447	0.81566	0.12665
6	CB	0.72775	0.90318	0.22712
7	CG	0.81323	0.71232	0.29498
8	CD1	0.72962	0.51447	0.33156
9	CE2	1.02179	0.49208	0.39648
10	CZ2	1.18841	0.42698	0.44798
11	CH2	1.33704	0.57796	0.43793
12	CZ3	1.31937	0.78498	0.37863
13	CE3	1.15347	0.84978	0.32755
14	CD2	1.00203	0.70184	0.33623
15	N	0.86779	0.74900	0.09384
16	NE1	0.85409	0.38144	0.39248
17	HO2	0.33321	0.48865	0.13462
18	HA	0.63075	0.96992	0.08283
19	H1	0.92523	0.58401	0.12225
20	H2	0.85062	0.72247	0.02488
21	H3	0.96026	0.89282	0.10754
22	HB1	0.59453	0.96505	0.24322
23	HB2	0.81288	1.07103	0.23019
24	HD1	0.58833	0.45648	0.31921
25	HE1	0.82644	0.23441	0.43032
26	HZ2	1.20060	0.26219	0.49376
27	HH2	1.46908	0.52868	0.47622
28	HZ3	1.43840	0.89571	0.37192
29	HE3	1.14332	1.01031	0.28121

ATOMS		DISTANCES	X	Y	Z	SYM	TRLN
2	4	1.1893	0.56695	0.59213	0.11089	1	555
3	4	1.3044	0.56695	0.59213	0.11089	1	555
3	17	0.9847	0.33321	0.48865	0.13462	1	555
4	2	1.1893	0.60052	0.40669	0.07084	1	555
4	3	1.3044	0.41729	0.63305	0.14558	1	555
4	5	1.5113	0.69447	0.81566	0.12665	1	555
4	17	1.8970	0.33321	0.48865	0.13462	1	555
5	4	1.5113	0.56695	0.59213	0.11089	1	555
5	6	1.5241	0.72775	0.90318	0.22712	1	555
5	15	1.4790	0.86779	0.74900	0.09384	1	555
5	18	1.1004	0.63075	0.96992	0.08283	1	555
6	5	1.5241	0.69447	0.81566	0.12665	1	555
6	7	1.4899	0.81323	0.71232	0.29498	1	555
6	22	1.0983	0.59453	0.96505	0.24322	1	555
6	23	1.0876	0.81288	1.07103	0.23019	1	555
7	6	1.4899	0.72775	0.90318	0.22712	1	555
7	8	1.3670	0.72962	0.51447	0.33156	1	555
7	14	1.4385	1.00203	0.70184	0.33623	1	555
8	7	1.3670	0.81323	0.71232	0.29498	1	555
8	16	1.3761	0.85409	0.38144	0.39248	1	555
8	24	1.0796	0.58833	0.45648	0.31921	1	555
9	10	1.3892	1.18841	0.42698	0.44798	1	555
9	14	1.4123	1.00203	0.70184	0.33623	1	555
9	16	1.3669	0.85409	0.38144	0.39248	1	555
10	9	1.3892	1.02179	0.49208	0.39648	1	555

10	11	1.	1.33704	0.57796	0.43793	1	555
10	26	1.	1.20060	0.26219	0.49376	1	555
11	10	1.3666	1.18841	0.42698	0.44798	1	555
11	12	1.3922	1.31937	0.78498	0.37863	1	555
11	27	1.0834	1.46908	0.52868	0.47622	1	555
12	11	1.3922	1.33704	0.57796	0.43793	1	555
12	13	1.3821	1.15347	0.84978	0.32755	1	555
12	28	1.0759	1.43840	0.89571	0.37192	1	555
13	12	1.3821	1.31937	0.78498	0.37863	1	555
13	14	1.3899	1.00203	0.70184	0.33623	1	555
13	29	1.0831	1.14332	1.01031	0.28121	1	555
14	7	1.4385	0.81323	0.71232	0.29498	1	555
14	9	1.4123	1.02179	0.49208	0.39648	1	555
14	13	1.3899	1.15347	0.84978	0.32755	1	555
15	5	1.4790	0.69447	0.81566	0.12665	1	555
15	19	1.0321	0.92523	0.58401	0.12225	1	555
15	20	1.0066	0.85062	0.72247	0.02488	1	555
15	21	1.0243	0.96026	0.89282	0.10754	1	555
16	8	1.3761	0.72962	0.51447	0.33156	1	555
16	9	1.3669	1.02179	0.49208	0.39648	1	555
16	25	0.9946	0.82644	0.23441	0.43032	1	555
17	3	0.9847	0.41729	0.63305	0.14558	1	555
17	4	1.8970	0.56695	0.59213	0.11089	1	555
18	5	1.1004	0.69447	0.81566	0.12665	1	555
19	15	1.0321	0.86779	0.74900	0.09384	1	555
19	20	1.6227	0.85062	0.72247	0.02488	1	555
19	21	1.6763	0.96026	0.89282	0.10754	1	555
20	15	1.0066	0.86779	0.74900	0.09384	1	555
20	19	1.6227	0.92523	0.58401	0.12225	1	555
20	21	1.6248	0.96026	0.89282	0.10754	1	555
21	15	1.0243	0.86779	0.74900	0.09384	1	555
21	19	1.6763	0.92523	0.58401	0.12225	1	555
21	20	1.6248	0.85062	0.72247	0.02488	1	555
22	6	1.0983	0.72775	0.90318	0.22712	1	555
22	23	1.7492	0.81288	1.07103	0.23019	1	555
23	6	1.0876	0.72775	0.90318	0.22712	1	555
23	22	1.7492	0.59453	0.96505	0.24322	1	555
24	8	1.0796	0.72962	0.51447	0.33156	1	555
25	16	0.9946	0.85409	0.38144	0.39248	1	555
26	10	1.0958	1.18841	0.42698	0.44798	1	555
27	11	1.0834	1.33704	0.57796	0.43793	1	555
28	12	1.0759	1.31937	0.78498	0.37863	1	555
29	13	1.0831	1.15347	0.84978	0.32755	1	555

ATOM B		A	ATOM C		D(BA)	D(AC)	ANGLE
4	(1 555)	3	17	(1 555)	1.304	0.985	111.17
2	(1 555)	4	3	(1 555)	1.189	1.304	125.54
2	(1 555)	4	5	(1 555)	1.189	1.511	123.44
2	(1 555)	4	17	(1 555)	1.189	1.897	96.59
3	(1 555)	4	5	(1 555)	1.304	1.511	111.01
3	(1 555)	4	17	(1 555)	1.304	1.897	28.95
5	(1 555)	4	17	(1 555)	1.511	1.897	139.96
4	(1 555)	5	6	(1 555)	1.511	1.524	113.11
4	(1 555)	5	15	(1 555)	1.511	1.479	108.44
4	(1 555)	5	18	(1 555)	1.511	1.100	106.87
6	(1 555)	5	15	(1 555)	1.524	1.479	111.24
6	(1 555)	5	18	(1 555)	1.524	1.100	109.13
15	(1 555)	5	18	(1 555)	1.479	1.100	107.83
5	(1 555)	6	7	(1 555)	1.524	1.490	115.20
5	(1 555)	6	22	(1 555)	1.524	1.098	106.06
5	(1 555)	6	23	(1 555)	1.524	1.088	107.33
7	(1 555)	6	22	(1 555)	1.490	1.098	111.46
7	(1 555)	6	23	(1 555)	1.490	1.088	110.01
22	(1 555)	6	23	(1 555)	1.098	1.088	106.31

6	(	1	555)	7	8	(	1	555)	1.490	1.367	127.53
6	(	1	555)	7	14	(	1	555)	1.490	1.438	126.48
8	(	1	555)	7	14	(	1	555)	1.367	1.438	106.00
7	(	1	555)	8	16	(	1	555)	1.367	1.376	110.32
7	(	1	555)	8	24	(	1	555)	1.367	1.080	129.62
16	(	1	555)	8	24	(	1	555)	1.376	1.080	120.06
10	(	1	555)	9	14	(	1	555)	1.389	1.412	122.27
10	(	1	555)	9	16	(	1	555)	1.389	1.367	130.12
14	(	1	555)	9	16	(	1	555)	1.412	1.367	107.62
9	(	1	555)	10	11	(	1	555)	1.389	1.387	117.01
9	(	1	555)	10	26	(	1	555)	1.389	1.096	120.93
11	(	1	555)	10	26	(	1	555)	1.387	1.096	122.06
10	(	1	555)	11	12	(	1	555)	1.387	1.392	121.26
10	(	1	555)	11	27	(	1	555)	1.387	1.083	118.40
12	(	1	555)	11	27	(	1	555)	1.392	1.083	120.32
11	(	1	555)	12	13	(	1	555)	1.392	1.382	121.67
11	(	1	555)	12	28	(	1	555)	1.392	1.076	119.01
13	(	1	555)	12	28	(	1	555)	1.382	1.076	119.31
12	(	1	555)	13	14	(	1	555)	1.382	1.390	118.35
12	(	1	555)	13	29	(	1	555)	1.382	1.083	120.38
14	(	1	555)	13	29	(	1	555)	1.390	1.083	121.27
7	(	1	555)	14	9	(	1	555)	1.438	1.412	107.15
7	(	1	555)	14	13	(	1	555)	1.438	1.390	133.40
9	(	1	555)	14	13	(	1	555)	1.412	1.390	119.44
5	(	1	555)	15	19	(	1	555)	1.479	1.032	113.42
5	(	1	555)	15	20	(	1	555)	1.479	1.007	111.87
5	(	1	555)	15	21	(	1	555)	1.479	1.024	110.26
19	(	1	555)	15	20	(	1	555)	1.032	1.007	105.48
19	(	1	555)	15	21	(	1	555)	1.032	1.024	109.20
20	(	1	555)	15	21	(	1	555)	1.007	1.024	106.26
8	(	1	555)	16	9	(	1	555)	1.376	1.367	108.91
8	(	1	555)	16	25	(	1	555)	1.376	0.995	125.97
9	(	1	555)	16	25	(	1	555)	1.367	0.995	125.03
3	(	1	555)	17	4	(	1	555)	0.985	1.897	39.88
15	(	1	555)	19	20	(	1	555)	1.032	1.623	36.72
15	(	1	555)	19	21	(	1	555)	1.032	1.676	35.24
20	(	1	555)	19	21	(	1	555)	1.623	1.676	58.98
15	(	1	555)	20	19	(	1	555)	1.007	1.623	37.81
15	(	1	555)	20	21	(	1	555)	1.007	1.625	37.24
19	(	1	555)	20	21	(	1	555)	1.623	1.625	62.15
15	(	1	555)	21	19	(	1	555)	1.024	1.676	35.55
15	(	1	555)	21	20	(	1	555)	1.024	1.625	36.50
19	(	1	555)	21	20	(	1	555)	1.676	1.625	58.86
6	(	1	555)	22	23	(	1	555)	1.098	1.749	36.64
6	(	1	555)	23	22	(	1	555)	1.088	1.749	37.06

END.

```
TEST OF SAI
7.407  5.3(     4.614     0.    -.15     0.
  29   2    . _.3            1          0.  01.  1.  1.     0   2
             1                2              3
            -1     .5         2             -3
CL          .958400 1.000000  .113391  .250000  .120180
   .01578
O1          .575000 1.000000  .600516  .406686  .070842
   .02058    .02198   .00507  -.00546   .00163  -.00290
O2          .575000 1.000000  .417291  .633052  .145583
   .01494    .03417   .00697  -.00529   .00220  -.00458
C           .662600 1.000000  .566946  .592134  .110891
   .01314    .01763   .00312  -.00326  -.00011  -.00027
CA          .662600 1.000000  .694474  .815664  .126655
   .01226
CB          .662600 1.000000  .727750  .903178  .227116
   .01309    .01500   .00287   .00248   .00036  -.00081
CG          .662600 1.000000  .813229  .712315  .294984
   .01250
CD1         .662600 1.000000  .729616  .514466  .331562
   .01465
CE2         .662600 1.000000 1.021785  .492077  .396484
   .01576
CZ2         .662600 1.000000 1.188407  .426982  .447981
   .01874
CH2         .662600 1.000000 1.337037  .577964  .437928
   .01618
CZ3         .662600 1.000000 1.319366  .784983  .378631
   .01331
CE3         .662600 1.000000 1.153465  .849778  .327547
   .01347
CD2         .662600 1.000000 1.002033  .701845  .336228
   .01263    .01725   .00223   .00021   .00117  -.00020
N           .950000 1.000000  .867793  .749001  .093844
   .01603    .02181   .00319  -.00301   .00184  -.00014
NE1         .950000 1.000000  .854089  .381441  .392481
   .01897
HO2        -.372000 1.000000  .333207  .488650  .134618
   .01737
HA         -.372000 1.000000  .630753  .969921  .082834
   .02204
H1         -.372000 1.000000  .925232  .584012  .122251
   .02017
H2         -.372000 1.000000  .850619  .722473  .024877
   .02569
H3         -.372000 1.000000  .960255  .892816  .107538
   .02064
HB1        -.372000 1.000000  .594533  .965052  .243218
   .02051
HB2        -.372000 1.000000  .812877 1.071033  .230190
   .02480
HD1        -.372000 1.000000  .588331  .456478  .319208
   .01857
HE1        -.372000 1.000000  .826438  .234407  .430316
   .02519    .03694   .00611  -.00515   .00211   .00672
HZ2        -.372000 1.000000 1.200600  .262188  .493763
   .02727    .03362   .00577   .00536   .00083   .00536
HH2        -.372000 1.000000 1.469077  .528678  .476218
   .02189
HZ3        -.372000 1.000000 1.438402  .895715  .371917
   .01738
HE3        -.372000 1.000000 1.143317 1.010307  .281212
   .02116
```

PROGRAM NAME	SCALER
PURPOSE	Wilson Plot and E's calculated
LIMITATIONS	
SWITCH SETTINGS	
LOGICAL UNITS	1 for input information CR is default
FILE ASSIGNMENTS	1 must be assigned if other than CR

SCALER

Program to compute the scale and temperature factors by Wilson's method and to compute |E|'s and obtain the associated statistics. The program may be recycled in order to refine the scale factor for the zonal reflections and the parity groups until the |E| statistics are satisfactory. For the recycling process, the weighting factors of the reflection class and parity group are varied. For the first two (2) cycles, the Wilson scaling is run. Thereafter, only the weighting factors are varied while the scale and temperature factors are not varied.

The reflection input for this program is the reflection file produced by MSRED. The input, other than the reflection data, is described below and is expected to be on logical unit 1, (the default device is the card reader).

INPUT:

1. TITLE (20A4)

2. KN2, KN3, KN4, KN5, KN6, DAMP(1), DAMP(2), EMIN (5I2, 3F6.2)

KN2	(0)/(1) - (normal)/(anisotropic temperature factor)
KN3	(0)/(1) - (do Wilson scaling)/(scale and temperature factors supplied)
KN4	(0)/(1) - (normal)/(replace F(obs) with unitary structure factor)
KN5	(0)/(1) - (do not list |E|)/(list reflections with |E| $\geq$ EMIN)
KN6	Number of cycles to be run. If KN3 = 0 and KN6 $\geq$ 2, 2 cycles of Wilson scaling will be run and remaining cycles will be concerned only with the weighting of the reflection classes and parity groups.
DAMP(1)	damping factor for change of reflection class weights (E). The default value is 0.4. A value of 1.0 disables the damping.
DAMP(2)	damping factor for change of parity group weights. The default value is 0.4. A value of 1.0 disables the damping.
EMIN	the minimum value of |E| to be listed if KN5 = 1.

3.* SCALE, TEMP, SCALA, TEMP1, TEMP2 (5F8.3)

(this card is <u>not</u> read if KN3 = 0)

4. (FNA(I), I = 1,10) (10F5.0)

FNA - no. of atoms having the scattering of type I atoms. Thus if on the file of reflection data, the order of form factors on the reflection record is 1-C, 2-N, 3-H and there are 20C, 16N and 36H atoms

20. 16. 36.

5. (ATME(I), I = 1,10) (10F5.0)

f(sin θ/λ = 0) for the corresponding atoms on the reflection record.

6. WG(I) - Epsilon values for the 7 reflections

WG(1) - E(psilon) for h k ℓ

WG(2) - E(psilon) for h k 0

WG(3) - E(psilon) for 0 k ℓ

WG(4) - E(psilon) for h 0 ℓ

WG(5) - E(psilon) for h 0 0

WG(6) 0 k 0

WG(7) 0 0 ℓ

default value for all E values is 1.0

7. WGP(I) - weighting for the 8 parity groups (8F5.0)

I	Group
1	ggg
2	ggu
3	gug
4	guu
5	ugg
6	ugu
7	uug
8	uuu

the default value is 1.0.

SCALER

8.* NR, IFA, IFB, AMIN, AMAX, FACT (3I5, 3F7.3)

NR - Number of sin θ/λ ranges for division of the data

IFA - (0)/(1)/(2) - (use all reflections as is)/(do not use unobserved data)/(use unobserved data with F(obs) multiplied by FACT)

IFB - 0

AMIN - minimum value of sin θ/λ to be included in scaling

AMAX - maximum value of sin θ/λ to be included in scaling

The data within AMIN and AMAX will be divided into equal volume elements in reciprocal space.

FACT - factor by which unobserved F(obs) values are to be multiplied

*This card is necessary only if KN3 = 0.

The card is read only once per run.

SCALER

Sample Input:

```
$*AS MT0:AJVUAC.DAT,7
$*AS KB:,1
$*RU SCALER
*AJVUAC WILSON PLOT -DATA LIST
* 0 0 0 4 0.4,0.4,0.0,
*14.,6.,4.,20.,
*6.,8.,7.,1.,
*
*
*15,0,0,.1,.6,1.0

A002 105540
$CO

$*FI
TIME:-11:39:59
CRYSNET 06-FEB-74
DOS V08-08
$*
```

← list all the E's

← ran out of paper

APPENDIX 2. CENTRAL SITE PROGRAM WRITEUPS

BNL CRYSTALLOGRAPHIC COMPUTER PROGRAM

PROGRAM ABSOR(INPUT,OUTPUT,PUNCH,TAPE6,TAPE4,TAPE3)

ABSOR IS A PROGRAM TO CALCULATE ABSORPTION CORRECTIONS FOR DATA FROM A 4-CIRCLE GONIOMETER BY THE ANALYTICAL METHOD OF DEMEULENAER AND TOMPA. IT IS A MAJOR REVISION OF THE PROGRAM AGNOST, BY L.TEMPLETON AND D.TEMPLETON AS DESCRIBED IN ABSTRACT E10, AMER.CRYST. ASSOC., STORRS,CONN.,1973.

MODIFIED FOR BNL INPUT, OUTPUT, DIFFRACTOMETER PARITY, AND DETERMINATION OF QUANTITIES NEEDED FOR EXTINCTION CALCULATIONS BY FLIEG HOLLANDER, JAN. 1975, AND PUT THROUGH *TIDY* TO BE CLEANED UP.

AN OVERVIEW OF THE ANALYTICAL METHOD FOR CALCULATION OF ABSORPTION CORRECTION IS GIVEN IN THE PAPER ANALYTICAL METHOD FOR ABSORPTION CORRECTION ,BY N.W.ALCOCK, WHICH APPEARS IN CRYSTALLOGRAPHIC COMPUTING , F.R. AHMED, ED., MUNKSGAARD, 1970, P.271.

THIS PROGRAM FOLLOWS THE BASIC OUTLINE GIVEN IN THE PAPER FOR BREAKING THE CRYSTAL UP INTO HOWELLS POLYHEDRA AND FOR CALCULATION OF THE ABSORPTION CORRECTION THEREAFTER. SEVERAL CHECKS HAVE BEEN BUILT INTO THE PROGRAM TO INSURE THE ACCURACY OF THE CALCULATION AND TO NOTE CASES WHERE THIS ACCURACY MAY HAVE BEEN COMPROMISED. SPECIFICALLY, THE VOLUME OF THE CRYSTAL AS DETERMINED DURING THE CALCULATION FOR A GIVEN REFLECTION IS COMPARED TO THE VOLUME CALCULATED INDEPENDENTLY, EARLY IN THE PROGRAM, TO BE SURE THAT ALL PARTS OF THE CRYSTAL HAVE MADE THEIR CONTRIBUTION TO THE ABSORPTION CORRECTION. REFLECTIONS FOR WHICH THERE IS AN ERROR OF 0.01 PERCENT OR GREATER IN COMPUTED VOLUME ARE FLAGGED IN THE PRINTED OUTPUT SO THAT THE USER CAN CHECK THEM.

THE ABSORPTION CORRECTION IS PASSED OUT OF THE PROGRAM AS A VARIABLE COR WHICH IS APPLIED AS A MULTIPLIER TO NETI IN PROGRAM CORDAT. E.G., CORRECTED INTENSITY = COR*NETI. THE ABSORPTION CORRECTION IS NOT APPLIED TO THE INTENSITY IN ABSOR.

THE PROGRAM ALSO CALCULATES QUANTITIES TO ALLOW FOR THE APPLICATION AND REFINEMENT OF ISOTROPIC AND ANISOTROPIC EXTINCTION CORRECTIONS IN FLINUS. THE QUANTITIES ARE TBAR, THE ABSORPTION WEIGHTED PATH LENGTH OF THE INCOMING AND OUTGOING BEAMS THROUGH THE CRYSTAL, AND THE COMPONENTS OF TWO VECTORS, XN AND XNSO, WHICH ARE USED FOR ANISOTROPIC EXTINCTION CORRECTIONS. (SEE P. COPPENS, EVALUATION OF ABSORPTION AND EXTINCTION... , P. 255 IN CRYSTALLOGRAPHIC COMPUTING .)

TBAR IS CALCULATED AS TBAR = -LN(FTRANS)/MU , WHERE FTRANS IS THE TRANSMISSION FOR THE GIVEN REFLECTION (=1.0/COR). THIS IS AN APPROXIMATION, BUT A REASONABLE ONE FOR MODERATE ABSORPTION. XN AND XNSO ARE TWO UNIT VECTORS WHICH ARE EXPRESSED AS THEIR COMPONENTS ALONG REAL CELL AXES OF UNIT LENGTH. XN IS PERPENDICULAR TO THE PLANE CONTAINING THE INCIDENT BEAM (VECTOR

SO) AND THE DIFFRACTED BEAM (VECTOR S). THE DIRECTION OF XN IS PARALLEL TO THE VECTOR (S X SO). XNSO IS A UNIT VECTOR PARALLEL TO (XN X SO). THUS XN, SO AND XNSO FORM A RIGHT-HANDED ORTHONORMAL VECTOR TRIPLE IN THAT ORDER. NOTE THAT THESE VECTORS DEPEND ON THE SPECIFIC SETUP USED FOR DATA COLLECTION AND THAT THEY MUST BE TRANSFORMED ALONG WITH THE H,K,L IF ANY CELL TRANSFORMATIONS ARE APPLIED AFTER DATA COLLECTION. ALSO NOTE THAT THEY WILL NOT BE THE SAME, IN GENERAL, FOR REFLECTIONS EQUIVALENT BY SYMMETRY. (SEE ALSO THE FLINUS WRITEUP.)

THE PROGRAM PERFORMS ITS CALCULATIONS IN PART USING A COORDINATE SYSTEM BASED ON THE DIFFRACTOMETER SETUP AND CRYSTAL ORIENTATION, WHICH MOVES WITH THE CRYSTAL. AS THIS SYSTEM IS DIFFERENT FOR THE DIFFERENT DIFFRACTOMETERS AT BNL, IT IS DESCRIBED IN SOME DETAIL BELOW.

FOR THE PICKER *XRAY* UNIT AND THE *MAIN* NEUTRON DIFFRACTOMETER THE COORDINATE SYSTEM WHICH IS RIGHT-HANDED AND MOVES WITH THE CRYSTAL IS AS FOLLOWS. WITH ALL SETTING ANGLES ZERO, X IS TOWARD THE BEAM SOURCE, Y IS COUNTERCLOCKWISE FROM X LOOKING DOWN ON THE HORIZONTAL PLANE , AND Z IS UP. FOR THESE MACHINES THE SENSES OF ROTATION OF THE ANGLES AT THE ZERO OF ALL ANGLES ARE , FOR THETA, OMEGA, PHI , Y GOES INTO X FOR + ROTATION ,FOR CHI , Z GOES INTO Y FOR + ROTATION. THIS GIVES NEGATIVE PARITY (SAME AS DEFINITION OF HAMILTON IN VOLUME FOUR OF INTERNATIONAL TABLES) FOR ALL THE ANGLES, AND AT TRUE CHI = 0.0 THE MACHINE POSITIONS THE CRYSTAL ABOVE THE GONIOMETER HEAD.

THE *SATT* NEUTRON DIFFRACTOMETER WORKS IN A LEFT-HANDED COORDINATE SYSTEM AT THE REACTOR. THIS IS CONVERTED TO A RIGHT-HANDED SYSTEM BY MANIPULATION OF THE U MATRIX (SEE CARDS 6). THE RIGHT-HANDED SYSTEM IS AS FOLLOWS. WITH ALL ANGLES AT TRUE ZERO, X IS TOWARDS THE SOURCE, Y IS CLOCKWISE FROM X LOOKING DOWN ON THE HORIZONTAL PLANE AND Z IS DOWN. FOR *SATT* THE SENSE OF ROTATION OF THE ANGLES AT ZERO OF ALL ANGLES IS AS FOLLOWS. FOR THETA, OMEGA, Y GOES INTO X FOR + ROTATION (NEG. PARITY). FOR PHI, X GOES INTO Y FOR + ROTATION (POS. PARITY). FOR CHI, Y GOES INTO Z FOR + ROTATION (POS. PARITY). AT TRUE CHI = 0.0 THE MACHINE HANGS THE CRYSTAL BELOW THE GONIOMETER HEAD. (WE NORMALLY WORK AT TRUE CHI NEAR 180 ON THIS MACHINE.)

****NOTE****

SEE ALSO THE WRITEUP FOR PROGRAM PROCK AND INPUT CARDS 6 BELOW FOR THE PROPER HANDLING OF *SATT* DATA.

****

***** TAPE FILES *****

TAPE3 IS LISTED RESULTS FOR ALL REFLECTIONS FOR OFF-LINE PRINTING.
FORMAT (3F4.0,F8.5,2F8.4,4F7.2,2I6,6F6.3,F8.4,F12.8)
H,K,L,TRANSMISSION, ABSORPTION CORRECTION (1/TRANS), NORMALIZING SCALE FACTOR, TWO THETA, OMEGA, CHI, PHI, NREF (FROM EXPT.), INTERNAL SERIAL NUMBER, COMPONENTS OF NORMALS, TBAR, VOLUME OF CRYSTAL AS CALCULATED FOR THAT PARTICULAR REFLECTION.

TAPE4 IS BCD OUTPUT, TO BE INPUT TO CORDAT.
FORMAT(3I3,2F10.1,F10.3,F7.4,2F7.2,2F3.0,2F8.0,I2,I6, 6F6.3,F8.5)
H,K,L,OBS,BAK,SCB,COR,PHI,CHI,SLO,SLB,OBS2,BAK2,ID,NREF, EXT,TBAR

COR IS THE ABSORPTION CORRECTION FACTOR TO BE APPLIED BY CORDAT. EXT IS A VECTOR CONTAINING THE COMPONENTS TO THE NORMALS USED FOR EXTINCTION CORRECTIONS AND TBAR IS THE ABSORPTION WEIGHTED PATH LENGTH. ALL OTHER VARIABLES ARE PASSED THROUGH ABSOR FROM PROCK. (SEE TAPE6)

TAPE6 IS INPUT TAPE AND IS OUTPUT FROM PROCK.
EITHER *SHORT* RECORDS, 80 CHARACTERS, WITH
FORMAT(3F3.0,2F10.1,F6.3,3F7.2,2F3.0,2F8.0,I2)
OR *LONG* RECORDS, 90 CHARACTERS, WITH
FORMAT (3F3.0,2F10.1,F10.3,3F7.2,2F3.0,2F8.0,I2,I6)
CONTAINING
H,K,L,OBS,BAK,SCB,OM,PHI,CHI,SLO,SLB,OBS2,BAK2,ID, AND IN THE CASE OF *LONG* RECORDS, NREF FROM THE EXPERIMENT.
SEE PROCK WRITEUP FOR DEFINITIONS OF VARIABLES.

****

***** INPUT CARDS *****

CARD 1 - (8A10) - TITLE

CARD 2 - (6F10.4) - REAL CELL PARAMETERS
A, B, C, AND ALPHA, BETA, GAMMA
OR COS(AL) OR COS(BET) OR COS(GAM)

CARD 3 - (I6I5) - ICN(16)
CONTROL INTEGERS.
ICN(1,2,7,10,12,15,16) ARE NOT USED AT PRESENT.

ICN(3) - COLUMN 15
APPLIES ONLY TO REFLECTIONS LISTED ON CARDS 7 OR IF PROGRAM IS ASKED TO CALCULATE ANGLES.
= 0, DATA COLLECTED IN BISECTING POSITION, OMEGA = 0.0 TRUE CHI IN FIRST OR FOURTH QUADRANT.
= 1, DATA COLLECTED IN PARALLEL POSITION, TRUE CHI = 90. TRUE OMEGA IN THIRD OR FOURTH QUADRANT.

ICN(4) - COLUMN 20
GENERATES THE CORRECT PARITIES FOR ANGLES ON BNL MACHINES.
APPLIES ONLY TO REFLECTIONS LISTED ON CARDS 7 OR IF PROGRAM IS ASKED TO CALCULATE ANGLES.
= 0, *MAIN* OR *XRAY* DIFFRACTOMETER.
= 1, *SATT* DIFFRACTOMETER USED.

ICN(5) - COLUMN 25
= 0, NO PUNCH OUTPUT
= 1, PUNCH OUT CARDS FOR ORTEP DRAWING OF CRYSTAL.

ICN(6) - COLUMN 26-30
= NFACES, NUMBER OF CRYSTAL FACES, SEE CARDS 8.

ICN(8) - COLUMN 40
= 0, CARD INPUT, SEE CARDS 10 BELOW.
= 1, TAPE6 INPUT FROM PROGRAM PROCK (SEE ABOVE).
= 2, TAPE6 INPUT FROM PROCK, *LONG* RECORDS CONTAINING REFLECTION NO. FROM THE EXPERIMENT.

ICN(9) - COLUMN 41-45
= N, SETTING ANGLES ARE CALCULATED FOR N REFLECTIONS, SEE CARDS 7 BELOW.

ICN(11) - COLUMN 51-55
= 0, NORMAL CASE.
= N, INCREMENT FOR SERIAL NO. OF REFLECTIONS. ICN(11) WILL BE ADDED TO THE SERIAL NO. READ FROM TAPE6 (IF ANY), AND INTERNALLY GENERATED SERIAL NUMBERS WILL START WITH N+1.

ICN(13) - COLUMN 65
= 0, PROGRAM CALCULATES ORIENTATION MATRIX, USE CARDS 5.
= 1, PUT IN ORIENTATION MATRIX, USE CARDS 6.

ICN(14) - COLUMN 70
= 0, CALCULATE ANGLES WITH THIS PROGRAM.
= 1, TAKE ANGLES FROM INPUT REFLECTIONS.

CARD 4 - (2F10.4) - WAVELENGTH, CHIZERO
WAVELENGTH IN ANGSTROMS.
CHIZERO NORMALLY= 0.0 SINCE WE READ IN TRUE ANGLES FROM PROCK. IT IS NEEDED ONLY IF WE ARE CALCULATING ANGLES FOR THE INPUT DATA (NOT THE CHECK CARDS).

CARDS 5 - USE ONLY IF ICN(I3) = 0 - (3F10.0,4F10.4) - 3 CARDS
H,K,L,TWOTHETA,OMEGA,CHI,PHI

TRUE VALUES OF SETTING ANGLES FOR THREE NON-COLINEAR REFLECTIONS. PROGRAM WILL USE THESE TO CALCULATE THE ORIENTATION MATRIX.

CARDS 6 - USE ONLY IF ICN(I3) = 1 - (3F10.7) - THREE CARDS
((U(I,J),J=1,3),I=1,3)

3 CARDS. EACH CARD CONTAINS ONE ROW OF THE U MATRIX AS PRINTED OUT BY THE COMPUTERS AT THE REACTOR. FOR *XRAY* AND *MAIN* THE U MATRIX SHOULD BE INPUT EXACTLY AS PRINTED. FOR *SATT* THE SIGNS OF THE ELEMENTS OF THE SECOND AND THIRD ROWS OF THE MATRIX SHOULD BE REVERSED FROM THE WAY THAT THEY ARE PRINTED OUT. SEE SUBROUTINE UMATRIC AND THE WRITEUP FOR PROGRAM PROCK.

CARDS 7 - SEE ICN(9) - (3F10.0,4F10.4)
H,K,L,TWOTHETA,OMEGA,CHI,PHI

TEST REFLECTIONS TO CHECK MATRIX CALCULATION OF ANGLES. THERE MUST BE EXACTLY ICN(9) CARDS IN THIS SET. IF ICN(9) = 0 DO NOT INPUT CARDS 7.

CARDS 8 - SEE ICN(6) - (3F10.0,F10.4) - H,K,L,D

H, K, L, ARE INDICES OF A CRYSTAL FACE AND D=DISTANCE IN CM FROM THAT FACE TO AN ORIGIN THAT MUST BE INSIDE THE CRYSTAL (D GREATER THAN 0.0). EXACTLY NFACES CARDS 8, ONE CARD FOR EACH BOUNDARY PLANE, MUST BE INPUT.

CARD 9 - (F10.6) - MU

MU = ABSORPTION COEFFICIENT IN 1.0/CM.

CARDS 10 - SEE ICN(8) - (3F3.0,2F10.1,F6.3,3F7.2,2F3.0,2F8.0,I2)
H,K,L,OBS,BAK,SCB,OM,PHI,CHI,SLO,SLB,OBS2,BAK2,ID

DATA INPUT ON CARDS. ID = 0 FOR DATA CARDS. ID = 2 TO TERMINATE READING OF DATA. SEE PROCK WRITEUP FOR DEFINITION OF VARIABLES.

05-MAR-75 AUTHOR: H. J. BERNSTEIN
23-MAY-76 REVISED: H. J. BERNSTEIN

ACCESS - 06/03/76

ACCESS

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

CDC CYBER 70/74, CDC CYBER 70/76
CDC SCOPE 3.4, CDC SCOPE 2.1

PURPOSE

ACCESS IS INTENDED TO PROVIDE A REPLACEMENT FOR THE REQUEST/STAGE CONTROL CARD, WHICH WILL COHERENTLY STAGE TAPE FILES INTO THE CATALOG. ACCESS CAN ALSO HANDLE COPIES FROM PRIVATE PACKS.

INTRODUCTION

ACCESS IS A FILE RETRIEVAL PROGRAM WRITTEN BY H. J. BERNSTEIN FOR SCOPE 3.4 AND SCOPE 2.1, COMBINING THE MAJOR FEATURES OF THE PROGRAMS ACCESS AND OBTAIN WRITTEN BY THE SAME AUTHOR FOR BNL SCOPE. THE EXTERNALS ARE SIGNIFICANTLY DIFFERENT. MOST RECORD MANAGER, PF, STAGE AND REQUEST CARD PARAMETERS ARE VALID. CONTROL CARDS MAY EXTEND OVER SEVERAL PHYSICAL CARDS. DIRECTORIES ARE FORMED FROM THE SAME PARAMETERS AS ARE USED ON THE CONTROL CARD. THE RECORD MANAGER IS USED FOR THE COPY LOGIC, SO MOST TAPE FORMATS CAN BE HANDLED. THE PROPER HANDLING FOR RANDOM FILES, HOWEVER, HAS NOT YET BEEN DETERMINED. UNFORTUNATELY, TAPES MAY NOT BE REQUESTED DIRECTLY FROM INTERCOM, SO ACCESS CANNOT BE USED INTERACTIVELY UNLESS THE FILE DESIRED IS ALREADY IN THE CATALOG. THUS THE INTERCOM USER IS OBLIGED TO TRY AN ACCESS, HAVE IT BOMB, AND THEN SUBMIT A BATCH JOB TO CREATE THE FILE, VIA ACCESS. UNLIKE THE SITUATION UNDER BNL SCOPE, SCOPE 3.4 JOBS MUST ALLOW FOR A MAGTAPE (MT1 OR NT1) ON THEIR JOB CARDS TO USE ACCESS.

05-MAR-75 AUTHOR: H. J. BERNSTEIN
23-MAY-76 REVISED: H. J. BERNSTEIN

ACCESS - 06/03/76

USE

ACCESS IS A CONTROL CARD OF THE FORM

```
ACCESS(FILE,PARAM1,PARAM2,...,PARAMN)
```

WHERE FILE IS THE NAME BY WHICH THE JOB IS TO USE THE FILE ACCESSED, AND EACH PARAMI IS OF ONE OF THE FOLLOWING FORMS.

```
KEYWORD
KEYWORD=VALUE
VALUE
```

THESE PARAMETERS COMBINE MOST OF THOSE USED ON ATTACH, CATALOG, FILE, STAGE, AND REQUEST CONTROL CARDS, AND HAVE SIMILAR MEANING.

IT IS IMPORTANT THAT A FILE CARD FOR THE FILE APPEAR BEFORE THE ACCESS CONTROL CARD, RATHER THAN AFTER, SINCE ACCESS MAY ACTUALLY WRITE THE FILE. THE FILE CARD PARAMETERS GIVEN ON THE ACCESS CONTROL CARD APPLY TO THE TAPE READ, NOT TO THE DISC FILE WRITTEN.

IF A DIRECTORY EXISTS IN THE SYSTEM CATALOG, THE USUAL USE IS

```
ACCESS(FILE,PFN=PFNAME,ID=IDNAME)
```

WHICH WILL ATTEMPT FIRST TO ATTACH THE FILE WITH THE NAME "PFNAME" AND THE ID "IDNAME", AND THEN WITH THE ID AS GIVEN, BUT WITH THE CHARACTERS "ZZG" PLACED IN FRONT. IF EITHER ATTACH WORKS, ACCESS EXITS. IF BOTH ATTACHES FAIL, THEN ACCESS WILL ATTEMPT TO ATTACH A DIRECTORY WITH PFN "IDNAME" AND ID "IDNAME". IF THAT FAILS A DIRECTORY OF ID AS GIVEN BUT WITH "ZZG" PLACED IN FRONT WILL BE USED. THE DIRECTORY SHOULD BE AN RT=Z, BT=C FILE OF CARD IMAGES CONTAINING ADDITIONAL ACCESS PARAMETERS TO IDENTIFY THE TAPE TO BE USED FOR THE FILES. THE PARAMETERS ARE MATCHED TO THE REQUESTED FILE BY SEARCHING FOR A MATCHING PFN AND ID.

AT PRESENT, ACCESS IS AVAILABLE AS A PERMANENT FILE BY ATTACH(ACCESS,ACCESS,ID=CPROGS) ON MFA, OR ATTACH(ACCESS,ACCESS,ID=ZZGCPROGS) ON MFZ. ACCESS IS NOT AVAILABLE ON MFB. IT WILL EXECUTE IN A VARIABLE FIELD LENGTH USUALLY LESS THAN 20K OCTAL. THE EXECUTION TIME VARIES GREATLY, DEPENDING ON EXACT FILE STRUCTURE.

THE PARAMETERS ON THE ACCESS CONTROL CARD ARE GIVEN BELOW.

THE FIRST GROUP OF PARAMETERS DEFINE THE TAPE FILE TO BE USED IF THE ATTACH FAILS.

```
DENSITY SETTING PARAMETERS
   HY  800 BPI, 7 TRACK
   HI  556 BPI, 7 TRACK
   LO  200 BPI, 7 TRACK
   PE 1600 BPI, 9 TRACK
   HD  800 BPI, 9 TRACK
DEFAULT IS HI


DEVICE TYPE
   MT  7 TRACK
   NT  9 TRACK
NOT NEEDED IF DENSITY IS GIVEN


CONVERSION CODE
   US  CONVERT FROM ASCII
   EB  CONVERT FROM EBCDIC
MEANINGFUL ONLY FOR 9 TRACK TAPE


STATION
   ST=GGG  STAGE FROM STATION GGG
MEANINGFUL ONLY ON CYBER 70/76
APPLIES ONLY TO THE TAPE FILE, NOT THE DISC.


VSN
   VSN=REEL  REEL NUMBER OF TAPE TO READ
USED AS DEFAULT FOR PFN


LABELING
   E, EXISTING LABELLED TAPE
DEFAULT IS UNLABELLED


NO RECOVERY
   NR  ACCEPT DATA WITH PARITY ERRORS
REFER TO SCOPE 2 REF MANUAL AND SCOPE 3.4 REF MANUAL
CAN CAUSE UNEXPECTED RESULTS
```

THE ABOVE PARAMETERS ARE USED TO FORM AN INTERNAL REQUEST OR STAGE FOR A FILE NAMED ZZZZZIN IN THE CASE THAT AN ATTACH FAILS. THIS FILE WILL BE COPIED TO THE FILE NAMED FILE, USING THE PARAMETERS BELOW TO DEFINE THE FILE CHARACTERISTICS OF THE TAPE. IF NONE OF THESE PARAMETERS ARE GIVEN, THE TAPE IS TREATED AS RT=S, BT=C, MBL=5120. THIS IS NOT THE STANDARD SCOPE 2.1 DEFAULT, AND CANNOT BE COPIED SAFELY TO A DEFAULT RT=W FILE, SO A FILE CARD WILL BE NEEDED.

05-MAR-75 AUTHOR: H. J. BERNSTEIN
23-MAY-76 REVISED: H. J. BERNSTEIN

ACCESS - 06/03/76

```
BLOCK TYPE
   BT=C  CHARACTER COUNT BLOCK, DEFAULT
   BT=K  RECORD COUNT
   BT=E  EXACT
   BT=I  INTERNAL CONTROL WORD
THESE AND OTHER FILE SPECIFICATION ARE FOR
THE TAPE ONLY.  THE DISK FILE IS WRITTEN AS
   RT=S,BT=C ON CYBER 70/74
   RT=W ON CYBER 70/76
WHICH MAY BE OVERRIDDEN BY A FILE CONTROL CARD


TRAILER COUNT
   CL=LENGTH (DECIMAL) FOR T FORMAT RECORDS
   CP=COUNT (DECIMAL)


CONVERSION MODE
   CM=YES  CONVERT CHARACTERS
   CM=NO  NO CONVERSION, DEFAULT


ERROR RECOVERY
   GOS  ALLOW 10 PARITY ERRORS
   GOS=NNN  ALLOW NNN PARITY ERRORS


RECORD LENGTH
   FL=NNN  LENGTH IN DECIMAL CHARACTERS


FILE ORGANIZATION - ALWAYS SEQUENTIAL
BUT THE DISC COPY MAY BE WORD ADDRESSABLE


T FORMAT HEADER
   HL=LENGTH  (DECIMAL)


D FORMAT LENGTH
   LL=LENGTH  (DECIMAL)


D FORMAT START
   LP=NNN


MAXIMUM BLOCK LENGTH
   MBL=NNN
DEFAULTS TO 5120


MAXIMUM RECORD LENGTH
   MRL=NNN
```

RECORDS PER BLOCK
RB=NNN

RECORD MARK CHARACTER
RMK=NNN

RECORD TYPE
RT=D DECIMAL CHARACTER COUNT
RT=F FIXED LENGTH
RT=R RECORD MARK
RT=S SCOPE LOGICAL, DEFAULT
RT=U UNDEFINED
RT=W CONTROL WORD
RT=Z ZERO BYTE

T FORMAT TRAILER
TL=NNN

THE USER MUST BE VERY CAREFUL TO CORRECTLY SPECIFY THE TAPE FILE CHARACTERISTICS WITH THE PARAMETERS ABOVE, AND THE DISC FILE CHARACTERISTICS WITH A FILE CARD APPEARING BEFORE THE ACCESS CONTROL CARD. UNFORTUNATELY, THE RECORD MANAGER CAN EXPEND A GREAT DEAL OF CP TIME TRYING TO COPY BADLY MATCHED RECORD TYPES. THE USER MUST BE ESPECIALLY CAREFUL TO SPECIFY RT=Z, BT=C, FL=NNN, RATHER THAN RT=S, WHEN TRYING TO WRITE A FILE OF LINE IMAGES FOR SCOPE 3.4, THOUGH IF BOTH TAPE AND DISC ARE RT=S, THE RESULTS WILL BE CORRECT. THE NEXT PARAMETERS ARE ALSO NEEDED IF HANDLING CODED 9 TRACK TAPES, SINCE THE RECORD MANAGER WILL IGNORE THE CONVERSION MODE WITHOUT THEM UNDER SCOPE 3.4.

SCOPE STRANGER TAPES AND LONG TAPES
S STRANGER TAPE (IGNORED ON 70/76)
L LONG TAPE (IGNORED ON 70/76)

THE NEXT GROUP OF PARAMETERS SPECIFY THE PERMANENT FILE TO BE ATTACHED AND/OR CATALOGED. WHEN NO DIRECTORY IS USED, THEY ARE NOT PARTICULARLY NEEDED. HOWEVER, ALL USERS SHOULD BE AWARE THAT ACCESS DEFAULTS TO MR=1, SO IF A FILE IS TO BE PURGED, THE PARAMETER MR= SHOULD BE SPECIFIED (A COMMA OR PERIOD DIRECTLY FOLLOWS THE MR=). ALTERNATIVELY, THE PARAMETER REPLACE MAY BE USED TO FORCE AN OLD COPY OUT, AND NOCOPY USED TO PREVENT A NEW CATALOG.

PERMANENT FILE NAME
PFN=NAME NAME TO USE FOR ATTACH AND CATALOG
DEFAULTS TO QQACCESSQQNNNNNNNNNNNNNNNNNNNNVSN
WHERE NNN... UNIQUELY IDENTIFIES THE FROM AND COPY
VALUES USED.

05-MAR-75
23-MAY-76

AUTHOR: H. J. BERNSTEIN
REVISED: H. J. BERNSTEIN

ACCESS - 06/03/76

ACCOUNT NUMBER
AC=ACCOUNT

CONTROL PASSWORD
CN=NAME

CYCLE NUMBER
CY=NNN

EXTEND PASSWORD
EX=NAME

USER IDENTIFICATION
ID=NAME
DEFAULT ID=TAPEFILES

LOWEST CYCLE NUMBER (ATTACH USE ONLY)
LC USE LOWEST CYCLE

MODIFY PASSWORD
MD=NAME

MULTIREAD ACCESS
MR

PRIVACY PROCEDURE
PP=NAME

PASSWORD
PW=NAME ONLY ONE PASSWORD AT A TIME

READ PASSWORD
RD=NAME

RETENTION PERIOD
RP=NNN
DEFAULTS TO ONE DAY

SETNAME
SN=NAME

TURNKEY PASSWORD
TK=NAME

EXCEPT READ
XR=NAME

NEW PFN
NPFN=NAME
ALLOWS A DIRECTORY MATCH TO CHANGE TO A NEW PFN

NEW ID
NID=NAME
ALLOWS A DIRECTORY ENTRY MATCHED TO CHANGE TO A NEW ID

DIRECTORY PFN
DPFN=NAME
DEFAULTS TO THE ID OF THE FILE ATTACHED

DIRECTORY ID
DID=NAME
DEFAULTS TO THE ID OF THE FILE ATTACHED

THE NEXT GROUP OF PARAMETERS ALLOW THE "TAPE" FILE TO BE ATTACHED FROM DISC.

SET "TAPE" FROM DISC
DISC
EQUIVALENT TO VSN=*******

TAPE ID
TID=NAME

TAPE SETNAME
TSN=NAME
IF THIS PARAMETER IS USED, THE JOB MUST CONTAIN A "MOUNT"

THE REMAINING PARAMETERS CONTROL THE DETAILED HANDLING OF THE SKIP AND COPY. IT SHOULD BE NOTED THAT, UNLIKE THE BNL SCOPE VERISON, THERE IS NO LEVEL NUMBER CONTROL. THE USER MUST SPECIFY THE TYPE OF COPY AND THE COUNT SEPARATELY. FOR EXAMPLE, COPYS,COPY=3, TO COPY THREE SECTIONS.

```
WAIT FOR BUSY FILE
   WAIT


SPECIFY FILE FROM TAPE TO COPY
   COPYP  COPY PARTITIONS
   COPYS  COPY SECTIONS
   COPYR  COPY RECORDS
   COPY=NNN COPY NNN OF THE UNITS SPECIFIED
   FROMP  SKIP PARTITIONS
   FROMS  SKIP SECTIONS
   FROMR  SKIP RECORDS
   FROM=NNN  SKIP NNN-1 OF UNITS SPECIFIED
DEFAULT IS TO COPY TO END OF INFORMATION, SKIPPING
PARTITIONS.  HOWEVER THE DEFAULT SKIP COUNT IS ZERO


USE PHYSICAL TAPE IF BUSY
   BUSY


USE PHYSICAL TAPE
   NOCOPY
MAKES ACCESS ACT LIKE A STAGE/REQUEST CARD
WHICH QUITS WITHOUT COPYING TO DISC


REPLACE EXISTING FILE
   REPLACE
IF FILE EXISTS, PURGE IT AND REPLACE IT


MAXIMUM SIZE OF FILE TO CATALOG
   SIZE=NNN
GIVEN IN CHARACTERS, DEFAULTS TO 5000000 ON CYBER 70/76
AND 1250000 ON CYBER 70/74


USE PREVIOUSLY REQUESTED/STAGED TAPE
   USETAPE
PREVENTS ACCESS FROM ATTEMPTING TO GET THE TAPE
THE USER MUST PROVIDE THE FILE ZZZZZIN.


CORRECT POSITION INFORMATION
   POS=NNN
PROVIDES ACCESS WITH THE ACTUAL CURRENT
POSITION OF ZZZZZIN.  THIS IS NEEDED WITH THE
USETAPE OPTION TO ALLOW ACCESS TO CORRECT THE
```

FROM INFORMATION (DEFAULT POS=1).

THE ABOVE TWO OPTIONS ALLOW ACCESS TO GET MULTIPLE FILES FROM ONE TAPE. POS SHOULD BE SET TO THE LAST FROM +1. NO DIRECTORY WILL BE USED.

USE A LOCAL FILE AS THE TARGET FOR THE COPY
USEDISC
PREVENTS ACCESS FROM ATTEMPTING EITHER AN ATTACH OR CATALOG OF THE FILE IT CREATES.

ACCESS USES THE PERMANENT FILE PARAMETERS GIVEN TO ATTEMPT AN ATTACH OF A COPY OF THE TAPE FILE FROM THE CATALOG, USING A PFN OF QQACCESSQQNNNNNNNNNNNNNNNNNNNNVSN IF NONE WAS GIVEN ON THE CONTROL CARD. IF THE ATTACH FAILS BECAUSE THE FILE DOES NOT EXIST, THE TAPE SPECIFIED IS REQUESTED AND COPIED INTO THE CATALOG, TO BE AVAILABLE FOR THE NEXT USE OF ACCESS. THE COPY USES THE RECORD MANAGER, WITH THE TAPE FILES DESCRIBED BY THE RECORD MANAGER FIELDS ON THE ACCESS CONTROL CARD, AND THE CATALOG FILE DESCRIBED BY A FILE CONTROL CARD, WHICH MUST APPEAR PRIOR TO THE ACCESS CARD.

IF NO REEL NUMBER IS GIVEN, AND THE FILE DOES NOT EXIST, ACCESS ATTEMPTS TO ATTACH A DIRECTORY FROM WHICH TO GET THE REEL NUMBER AND OTHER DATA. THE DIRECTORY MUST BE AN RT=Z, BT=C FILE WITH CARD IMAGES OF THE MISSING INFORMATION IN COLUMNS 1 THROUGH 72 OF EACH CARD, STARTING WITH PFN=NAME, AND TERMINATED BY A PERIOD. ANY FIELD GIVEN IN THE DIRECTORY OVERRIDES THE SAME FIELD IN THE CONTROL CARD. THE DIRECTORY APPEARS AS PACKETS OF CARDS, EACH BEGINNING WITH PFN=NAME, SO THAT NAME MATCHES THE NAME OF THE PERMANENT FILE TO BE ACCESSED. IF THE ID OF THE FILE IS NOT TAPEFILES, THE ID=NAME PARAMETER MUST APPEAR BOTH ON THE CONTROL CARD AND IN THE DIRECTORY. FIELDS IN THE DIRECTORY PACKETS ARE OF EXACTLY THE SAME FORM AS THOSE ON THE CONTROL CARD, AND MAY CONTINUE OVER AS MANY CARDS AS ARE NEEDED, EXCEPT, UNLIKE THE CONTROL CARD, ONLY COLUMNS 1-72 ARE SCANNED. NO FIELD MAY CROSS FROM COLUMN 72 OF ONE CARD TO COLUMN 1 OF THE NEXT. IF THAT OCCURS, ONLY THE PORTION ON THE SECOND CARD WILL BE USED.

MESSAGES

ALL OPERATING SYSTEM MESSAGES HAVING TO DO WITH TAPE I/O AND CATALOG USE MAY APPEAR. IN ADDITION, ACCESS ISSUES THE FOLLOWING MESSAGES.

UT000 - ILLEGAL PARAMETER - NNNNNN CONTENTS
IS ISSUED WHEN ACCESS DETECTS AN INVALID FIELD IN THE CONTROL CARD OR DIRECTORY. NNNNNN IS THE FIELD NUMBER, AND CONTENTS ARE THE CONTENTS OF THE FIELD IN ERROR. FAILURE TO USE AN = ON A KEYWORD REQUIRING IT OFTEN CAUSES THIS ERROR.

UT023 - ACCESS TERMINATED
IS ISSUED JUST BEFORE THE ABNORMAL TERMINATION OF ACCESS FOR ANY REASON. PRIOR MESSAGES SHOULD CONTAIN THE REASON.

UTC00 - DIRECTORY REQUIRED
IS ISSUED WHEN ACCESS HAS INSUFFICIENT INFORMATION TO LOCATE THE FILE AND MUST ATTACH A DIRECTORY. IF THE DIRECTORY IS NOT THERE, THIS MESSAGE WILL BE FOLLOWED BY AN ABORT BY THE OPERATING SYSTEM.

UTC01 - NNNNNNNNNN CHARS WRITTEN
GIVES THE DECIMAL NUMBER OF CHARACTERS WRITTEN BY ACCESS TO THE DISC.

UTC02 - FILE CATALOGED
IS ISSUED BY ACCESS AFTER THE DISC FILE HAS BEEN PLACED IN THE CATALOG.

UTC03 - FILE NOT IN DIRECTORY
IS ISSUED WHEN ACCESS WAS ABLE TO ATTACH THE DIRECTORY, BUT COULD NOT LOCATE THE DESIRED PFN AND ID.

PFNNN - PERMANENT FILE ACTION ERROR
REPORTS THE FAILURE OF THE ACCESS ATTEMPT TO ATTACH THE FILE WITHOUT A TAPE COPY. NNN IS THE ERROR STATUS RETURNED BY THE SYSTEM. ANYTHING OTHER THAN PF012 OR PF025 WILL BE FOLLOWED BY AN ABORT.

UT020 - RT=U MUST HAVE BT=K,RB=1

UT021 - UNIDENTIFIED DATA EXIT TAKEN

UT030 - COPY COMPLETE

UT031 - EOI ENCOUNTERED

UT032 - EOP ENCOUNTERED

UT033 - EOS ENCOUNTERED

UT034 - RECORDS/SECTIONS/PARTITIONS - NN NN NN
REPORTS THE TOTAL DATA TRANSFER IN SKIPS AND COPIES

UT037 - ERROR WHILE COPYING --

RMNNN - ERROR ON FILE NAMED XXXXXXX
REPORTS A RECORD MANAGER ERROR NUMBER NNN WHICH ABORTS ACCESS.

UT200 - DATA IS LEFT JUSTIFIED, ZERO FILLED

UT201 - EXCESS DATA WILL BE TRUNCATED

UT202 - F/R/Z DATA TRUNCATED

UT203 - FILE IS NOT SEQUENTIAL

UT204 - LIBRARY COPY MAY BE LESS THAN ONE PARTITION

THE UNDETAILED MESSAGES ABOVE ARE THE SAME AS FOR THE SCOPE 2 COPY UTILITIES.

EXAMPLE

TO ACCESS THE THIRD FILE ON A TAPE OF SCOPE 2 BINARIES WRITTEN IN THE SYSTEM DEFAULT RT=W FORMAT, THE FOLLOWING ACCESS CONTROL CARD WOULD WORK.

```
ACCESS(FILE,VSN=X1234,RT=W,BT=I,MBL=5120,
COPYP,FROM=3)
```

NOTE THAT THE COPYP WAS NEEDED TO FORCE A COPY OF JUST ONE FILE AND THAT THE RT=W WAS NEEDED SINCE THE DEFAULT TAPE FORMAT ASSUMED BY ACCESS IS RT=S.

IF INSTEAD WE WISHED TO USE A DIRECTORY AND FIND THIS SAME FILE BY NAME, WE WOULD FIRST HAVE TO CATALOG A DIRECTORY, SAY BY THE FOLLOWING JOB

```
JOB CARD ...
ACCOUNT CARD ...
```

05-MAR-75
23-MAY-76

AUTHOR: H. J. BERNSTEIN
REVISED: H. J. BERNSTEIN


```
REQUEST,DIR,*PF.
FILE(DIR,RT=Z,BT=C,FL=80)
COPYBF(INPUT,DIR)
REWIND,DIR.
CATALOG(DIR,DIR,ID=DIR,AC=NNN,RP=999,XR=DIR)
7/8/9
PFN=MYNAME,ID=DIR,
VSN=X1234,RT=W,BT=I,MBL=5120,COPYP,FROM=3.
6/7/8/9
```

AFTER WHICH THE FILE WILL BE AVAILABLE BY

```
ACCESS(FILE,PFN=MYNAME,ID=DIR)
```

WHICH WILL EITHER ATTACH THE FILE, OR IF IT IS NOT THERE READ THE DIRECTORY DIR, FIND THE TAPE INFORMATION AND COPY THE FILE INTO THE CATALOG.

I N D E X

ACCOUNT NUMBER ACCESS-6
  AC=ACCOUNT ACCESS-6
BLOCK TYPE ACCESS-4
  BT=C - CHARACTER COUNT ACCESS-4
  BT=E - EXACT ACCESS-4
  BT=I - INTERNAL ACCESS-4
  BT=K - RECORD COUNT ACCESS-4
CONTROL PASSWORD ACCESS-6
  CN=NAME ACCESS-6
CONVERSION CODE ACCESS-3
  EB - EBCDIC ACCESS-3
  US - ASCII ACCESS-3
CONVERSION MODE ACCESS-4
  CM=NO ACCESS-4
  CM=YES ACCESS-4
CYCLE NUMBER ACCESS-6
  CY=NNN ACCESS-6
DENSITY SETTING PARAMETERS
  ACCESS-3
  HD - 800 BPI ACCESS-3
  HI - 556 BPI ACCESS-3
  HY - 800 BPI ACCESS-3
  LO - 200 BPI ACCESS-3
  PE - 1600 BPI ACCESS-3
DEVICE TYPE ACCESS-3
  MT - 7 TRACK ACCESS-3
  NT - 9 TRACK ACCESS-3
DIRECTORY ACCESS-2
DIRECTORY ID ACCESS-7
  DID=NAME ACCESS-7
DIRECTORY PFN ACCESS-7
  DPFN=NAME ACCESS-7
D FORMAT LENGTH ACCESS-4
  LL=LENGTH ACCESS-4
D FORMAT START ACCESS-4
  LP=NNN ACCESS-4
ERROR RECOVERY ACCESS-4
  GOS ACCESS-4
  GOS=NNN ACCESS-4
EXAMPLE ACCESS-11
EXCEPT READ PASSWORD ACCESS-7
  XR=NAME ACCESS-7
EXTEND PASSWORD ACCESS-6
  EX=NAME ACCESS-6
FILE FROM TAPE TO COPY ACCESS-8
  COPYP - COPY PARTITIONS ACCESS-8
  COPYR - COPY RECORDS ACCESS-8
  COPYS - COPY SECTIONS ACCESS-8
  COPY=NNN - COPY NNN UNITS
    ACCESS-8
  FROMP - SKIP PARTITONS ACCESS-8
  FROMR - SKIP RECORDS ACCESS-8
  FROMS - SKIP SECTIONS ACCESS-8
  FROM=NNN - SKIP NNN-1 UNITS
    ACCESS-8
  POS=NNN - CURRENT POSITION
    ACCESS-8
FILE ORGANIZATION ACCESS-4
INTRODUCTION ACCESS-1
LABELING ACCESS-3
  E - EXISTING ACCESS-3
LOCAL DISC FILE ACCESS-9
  USEDISC ACCESS-9
LOWEST CYCLE NUMBER ACCESS-6
  LC ACCESS-6
MAXIMUM BLOCK LENGTH ACCESS-4
  MBL=LENGTH ACCESS-4
MAXIMUM RECORD LENGTH ACCESS-4
  MRL=NNN ACCESS-4
MAXIMUM SIZE OF FILE ACCESS-8
  SIZE=LENGTH ACCESS-8
MESSAGES ACCESS-10
MODIFY PASSWORD ACCESS-6
  MD=NAME ACCESS-6
MULTIREAD ACCESS ACCESS-6
  MR ACCESS-6
NEW ID ACCESS-7
  NID=NAME ACCESS-7
NEW PFN ACCESS-7
  NPFN=NAME ACCESS-7
NO RECOVERY ACCESS-3
  NR ACCESS-3
PASSWORD ACCESS-6
  PW=NAME ACCESS-6
PERMANENT FILE NAME ACCESS-5
  PFN=NAME ACCESS-5
PHYSICAL TAPE IF BUSY ACCESS-8
  BUSY ACCESS-8
  NOCOPY ACCESS-8
PRIVACY PROCEDURE ACCESS-6
  PP ACCESS-6
PURPOSE ACCESS-1
READ PASSWORD ACCESS-6
  RD ACCESS-6
RECORDS PER BLOCK ACCESS-5
  RB=NNN ACCESS-5
RECORD LENGTH ACCESS-4
  FL=LENGTH ACCESS-4
RECORD MARK CHARACTER ACCESS-5
  RMK=NNN ACCESS-5
RECORD TYPE ACCESS-5
  RT=D - DECIMAL CHARACTER COUNT
    ACCESS-5
  RT=F - FIXED LENGTH ACCESS-5
  RT=R - RECORD MARK ACCESS-5
  RT=S - SCOPE LOGICAL ACCESS-5
  RT=U - UNDEFINED ACCESS-5
  RT=W - CONTROL WORD ACCESS-5
  RT=Z - ZERO BYTE ACCESS-5
REPLACE EXISTING FILE ACCESS-8

RETENTION PERIOD ACCESS-6
RP=NNN ACCESS-6
SCOPE STRANGER TAPES AND LONG TAPES
ACCESS-5
L - LONG ACCESS-5
S - STRANGER ACCESS-5
SETNAME ACCESS-6
SN=NAME ACCESS-6
SET "TAPE" FROM DISC ACCESS-7
DISC ACCESS-7
STATION ACCESS-3
ST=GGG ACCESS-3
TAPE ID ACCESS-7
TID=NAME ACCESS-7
TAPE PFN ACCESS-7
TPFN=NAME ACCESS-7
TAPE SETNAME ACCESS-7
TSN=NAME ACCESS-7
TRAILER COUNT ACCESS-4
CL=LENGTH ACCESS-4
CP=COUNT ACCESS-4
TURNKEY PASSWORD ACCESS-7
TK=NAME ACCESS-7
T FORMAT HEADER ACCESS-4
HL=LENGTH ACCESS-4
T FORMAT TRAILER ACCESS-5
TL=LENGTH ACCESS-5
USE ACCESS-2
USER IDENTIFICATION ACCESS-6
ID=NAME ACCESS-6
USE STAGED OR REQUESTED FILE
ACCESS-8
USETAPE ACCESS-8
VSN ACCESS-3
VSN=REEL ACCESS-3
WAIT FOR BUSY FILE ACCESS-8

```
      PROGRAM AVBANG (INPUT,OUTPUT)
C
C
C
C     NAME:      AVBANG
C     AUTHOR:    T KOETZLE BNL
C     DATE:      SEPT 73
C     MACHINE:   CDC 6600
C     COMPILER:  FTN
C
C*********************************************************************
C                                                                    *
C     CALCULATION OF MEAN VALUES AND VARIANCES FROM A SAMPLE POPULATION *
C                                                                    *
C*********************************************************************
C                                                                    *
C     INPUT                                                          *
C                                                                    *
C     CARD    1  (9A6)                    TITLE CARD                 *
C                COLS  1-54    TITLE      ANY ALPHANUMERIC INFORMATION *
C                                                                    *
C     CARD    2  (9A6)                    SAMPLE IDENTIFIER          *
C                COLS  1-54    PARAM      ANY ALPHANUMERIC INFORMATION *
C                COLS  1- 4               PUNCH STOP TO TERMINATE JOB *
C                                                                    *
C     CARD    3  (10F6.3)                 SAMPLE POPULATION          *
C                COLS  1- 6    X(1)       MEASUREMENT                *
C                COLS  7-12    S(1)       ESTIMATED STANDARD DEVIATION *
C                COLS 13-18    X(2)       MEASUREMENT                *
C                COLS 19-24    S(2)       ESTIMATED STANDARD DEVIATION *
C                                        AND SO ON                  *
C                                                                    *
C*********************************************************************
C                                                                    *
C     INCLUDE AS MANY CARDS 3 AS NECESSARY FOR EACH SAMPLE POPULATION *
C     TERMINATE EACH SUCH POPULATION WITH X(I) BLANK                 *
C     FOLLOW BY A NEW CARD 2 AND SO ON                               *
C                                                                    *
C     AN OBSERVATION WITH S(I) NEGATIVE WILL BE IGNORED              *
C                                                                    *
C*********************************************************************
C                                                                    *
C     OUTPUT                                                         *
C                                                                    *
C     INPUT MEASUREMENTS AND ESTIMATED STANDARD DEVIATIONS           *
C     RANGE AND NUMBER OF OBSERVATIONS                               *
C     XBAR = MEAN VALUE = SUM(X(I))/NOBS                             *
C     SIGMA OF POPULATION = SQRT(SUM((X(I)-XBAR)**2)/(NOBS-1))       *
C     SIGMA OF MEAN = SIGMA OF POPULATION/SQRT(NOBS)                 *
C     WXBAR = WEIGHTED MEAN VALUE = SUM(X(I)/S(I)**2)/SUM(1./S(I)**2) *
C     EXTERNAL SIGMA OF WEIGHTED MEAN =                              *
C     SQRT(SUM((X(I)-WXBAR)**2/S(I)**2)/(SUM(1./S(I)**2)*(NOBS-1)))  *
C                                                                    *
C*********************************************************************
```

NAME: AVSORT

AUTHOR: G.J.B. Williams (most recently)

CORE: $10K_8$ + $NOBS_8$ (more than 40K if subroutines are replaced)

DATE: December 1974

ECS: $(6 * NOBS)_8$

PROGRAM AVSORT (INPUT,ØUTPUT,TAPE1,DATA,TAPE3,SHØRT1,TAPE2=DATA,TAPE4=SHØRT1, TAPE5=INPUT,TAPE6=ØUTPUT)

I. PURPOSE:

Sorting and averaging of equivalent reflection amplitudes.

II. FILES:

A. TAPE1-BCD or binary Purpose-input

B. DATA-Binary Purpose-output to be used in LINUS

C. TAPE3-BCD Purpose-output

III. LIMITATIONS:

24999 reflections
$-50 \leq$ any Miller index ≤ 49
300 equivalent members of a form
20 index triples to exclude from agreement factors.

IV. REPLACEABLE SUBROUTINES:

	Arguments
A. IMP-reads BCD or binary tape for input.	IDENT,FH,FK,FL,SF,WEIGHT,SCALEN, E1,E2,E3,E4,E5,E6,E7,ICN
B. REJECT-rejects systematic absences.	FH,FK,FL,IREJ
C. SPACE-transforms indices.	FH,FK,FL
D. FORM-checks indices for correct member of form	IFORM,H(3 elements)

V. DECK SET UP

A. JOB CARD
1. TIME LIMIT - 3 minutes (try 200_8 seconds)
2. FIELD LENGTH - $40K_8$ + $NOBS_8$ + $\sim 10K_8$ for subroutines
3. NUMBER OF TAPES - 0-3
4. ECS or LCM - $(6 * NOBS)_8$

B. CONTROL CARDS

```
FTN(SYSEDIT) if using subroutines
ATTACH(AVGE,AVSORT,ID=CPROGS)
REQUEST(TAPE1,,,,)          NOTE: input tape.  (only if needed)
REQUEST(DATA,,,,)           NOTE: output tape, binary (only if needed)
REQUEST(TAPE3,,,,)          NOTE: BCD output.  (only if needed)
LØAD(LGØ).  if using subroutines
AVGE.
```

C. DATA CARDS:

CARD	FORMAT (no. of variables indicated by no. of fields)
1. Title card	8A10
2. Cell constants	7F9.6
3. Control card 1 (systematic absences)	12I5
4. Limit card	(6F5.0,2F10.5)
5. Control card 2 (concordance limits)	(4F10.5)
6. Control card 3 (option selection)	(9I5)
7. Indices to exclude from agreement factors (if needed)	(3I5)
8. Reflection data if data is input on cards	(I1,F3.0,2F4.0,F11.3,F10.3,F3.0,6F6.3,F8.5)
9. Terminator	(as above but this card is not necessary,-- if it is supplied it should have a 1 in cc 1.)

D. SUMMARY FILES:

1. SHØRT1

Brookhaven Crystallographic Computer Program

NAME: AVSORT TIME: very fast (see Example)

CORE FL: 40K + $NOBS_8$

ECS FL: $(6 * NOBS)_8$

Purpose: Sorting, averaging of equivalent reflection intensities (either F or F**2) and sigmas, and general preparation of reflection data for further analysis. For description of program and restrictions on redimensionable arrays, see Method.

AVSORT supersedes program ECSORTH.

PROGRAM AVSORT (INPUT,ØUTPUT,TAPE1,DATA,TAPE3,SHØRT1,TAPE2=DATA,TAPE4=SHØRT1,TAPE5=INPUT,TAPE6=ØUTPUT)

Input Data:

1. (8A10) TITLE will appear as first record on OUTPUT and SHORT1.
2. (7F9.6) (RCP(I),I=1,6) reciprocal cell constants, (a*,b*,c*,cosα*,cosβ*,cosγ*)
   ELAMBA wavelength in Angstroms

   NOTE if the user is employing either subroutine IMP or SPACE to transform his/her indices to those which correspond to a different unit cell from that used in data collection then he must input the cell parameters for the NEW cell here. This is because the program calculates sinθ for both the input and generated (during the search phase) indices to check against the limits see below.

3. (12I5) Control Card 1.

   col. 1- 5 NOBS .GE. total number of reflections input on TAPE1 or on cards.

   6-10 IUN = 0, normally (only the input reflections are considered)
   = 1, for inclusion of unmeasured (i.e., reflections acceptable but not in input list), in order, on the output file(s) (see Method).

   Following specify the moduli of the h,k,ℓ of the unmeasured reflections permissible (acceptable for the user's space group). These tests are applied only if there are no measurements of an index triple and IUN ≠ 0.

   11-15 IHK = 0, all orders permissible.
   = 1, h+k = 0(mod 2), permissible for hkℓ

   16-20 IHL = 0, a.o.p.
   = 1, h+ℓ =0(mod 2), permissible for hkℓ

21-25	IKL	= 0, a.o.p. = 1, $k+\ell = 0 \pmod 2$, permissible for $hk\ell$
26-30	IHKL	= 0, a.o.p. = 1, $h+k+\ell = 0 \pmod 2$, permissible for $hk\ell$
31-35	IHKO	= 0, a.o.p. = 1, $h+k = 0 \pmod 2$ permissible for $hk0$ = 2, $h = 0 \pmod 2$, permissible for $hk0$ = 3, $k = 0 \pmod 2$, permissible for $hk0$
36-40	IHOL	= 0, a.o.p. = 1, $h+\ell = 0 \pmod 2$, permissible for $h0\ell$ = 2, $h = 0 \pmod 2$, permissible for $h0\ell$ = 3, $\ell = 0 \pmod 2$, permissible for $h0\ell$
41-45	IOKL	= 0, a.o.p. = 1, $k+\ell = 0 \pmod 2$, permissible for $0k\ell$ = 2, $k = 0 \pmod 2$, permissible for $0k\ell$ = 3, $\ell = 0 \pmod 2$, permissible for $0k\ell$
46-50	IH	= 0, a.o.p. = 1, $h = 0 \pmod 2$, permissible for $h00$
51-55	IK	= 0, a.o.p. = 1, $k = 0 \pmod 2$, permissible for $0k0$
56-60	IL	= 0, a.o.p. = 1, $\ell = 0 \pmod 2$, permissible for 00ℓ

NOTE the tests provided do not comprise an exhaustive list of the possible systematic extinction conditions. Tests not given here may be programmed into SUBROUTINE REJECT which is called, for EVERY generated triple between the sinθ limits, before the above systematic absence information is applied. If IUN=1 then ALL reflections which are between the index limits, can pass the above tests, and not excluded by REJECT will appear on the output file. In high symmetry groups this implies that both $hk\ell$ and $kh\ell$ (for example) will be output.

4. (6F5.0,2F10.5)

col.			
	1-5	XHL	H index lower limit
	6-10	XHU	H index upper limit
	11-15	XKL	K index lower limit
	16-20	XKU	K index upper limit
	21-25	XLL	L index lower limit
	26-30	XLU	L index upper limit
	31-40	XSINTL	sin(THETA) lower limit
	41-50	XSINTU	sin(THETA) upper limit

If ALL of XHL thru XLU are input as zero (blank) then the program will determine the search limits internally from the extreme values returned by subroutine SPACE. See METHOD if you plan to input these values.

If BOTH of XSINTL and XSINTU are input as zero (or blank) then these variables are reset to 0.0001 and 1.0 respectively.

5. (3F10.5)

col.	1-10	C1	Not currently in use.
	11-20	C2	Maximum allowable deviation, expressed as multiples (fractions) of the individual sigmas.
	21-30	C3	Maximum allowable deviation, expressed as a fraction of the <u>estimated deviation of an individual reflection</u> from FMEAN.
	31-40	C4	Fractional non-Poisson contribution to the variance (see below). Used only in the concordance testing.

All values for C_1, C_2, or C_3 input less than or equal to 0.0 are reset to 999.99.

The above 3 parameters are used to test for significant deviations of any one determination from the unweighted mean of all the contributors.

If we define:

$\bar{F} = (\sum F_i)/n$ i.e. the simple mean

$\Delta = |\bar{F}-\bar{F}_i|$ i.e. the deviation for any one value

$\sigma_{<F>}$ = the standard deviation of the mean as derived from the input σ's for individual observations plus non-Poisson contributions as specified by C4.

$\sigma_S = ((\sum|\bar{F}-F_i|^2)/n)^{\frac{1}{2}}$ i.e. the estimated standard deviation of an individual reflection as determined from the spread of the contributors to $\bar{F}$

A. If there are <u>TWO OR MORE CONTRIBUTORS</u> to $\bar{F}$ the tests, and the order in which they are applied, are:

(i) if $\Delta \geq C_1.\bar{F}$ reject F_i <u>Note</u> Test (i) is no longer applied.

(ii) if $\Delta \geq C_2.\sigma_{<F>}$ reject F_i

(iii) if $\Delta \geq C_3.\sigma_S$ reject F_i

Rejected measurements are flagged with 2 or 3 asterisks on the printed output depending upon which test they failed. If, because of bad data or overly stringent criteria, all contributors to a form are rejected then the program will recalculate $\bar{F}$ and σ_S excluding the datum with the largest $|\bar{F}-F_i|$ and recycle through the contributors bypassing the excluded measurement. Only one such recycling will occur.

B. If there are TWO OR MORE contributors then a modified $\sigma_{<F>}$ is formed as defined by $\sigma_{<F>}^2 = 1/n\sum(\sigma_i^2 + C_4^2F_i^2)$ and it is this $\sigma_{<F>}$ which is used in test (ii) above. Two reflections are counted as /DISPARATE DOUBLY DETERMINED/ if either determination deviates by more than $C_2\sigma_{<F>}$ from the unweighted mean.

C. If there is only ONE DETERMINATION for a reflection then Δ=0.0 and the reflection will pass all three tests above. THERE ARE NO STATISTICAL TESTS IN THIS PROGRAM WHICH WILL PASS JUDGEMENT ON THE FITNESS OF A REFLECTION AS LEAST-SQUARES INPUT.

6. (9I5)

Col	1-5	ICN	denotes source of the reflection data. = 1 implies data on cards--see INPUT below = 2 read card images from file TAPE1 = 3 unformatted records from file TAPE1
	6-10	IBCD	= 0 do not write coded output file TAPE3--see OUTPUT below > 0 write processed data in coded form to TAPE3
	11-15	IBNRY	≤ 0 do not write unformatted file DATA > 0 write unformatted information to DATA
	16-20	IPRNT	= 0 do not list reflections on OUTPUT > 0 produce full listing on OUTPUT
	21-25	NEXCL	This is the number of reflections (≤20) which the user wishes to exclude from the agreement factor calculations. The monitor reflections should be excluded to avoid biasing the statistics
	26-30	ISF	This integer may be used to distinguish data batches which are to be merged later. For reflections to which there corresponds at least one measurement the ISF value is simply transferred to the output media. For the unmeasured (synthetic) reflections a dummy value of 99 is output. FLINUS uses this integer as a scale factor number and so a positive value (usually 1) should be used.
	31-35	JORDH	These three integers specify the order in which the user wants the data sorted. The index with order indicator 1 will vary most rapidly in the final outputs; 2 will denote the index of intermediate acceleration and 3 the least rapidly varying.
	36-40	JORDK	
	41-45	JORDL	

7. (3I5) OMIT IF NEXCL = 0.

Col	1-5	KEXCL(I,1)	There should be NEXCL of these cards, each bearing the indices of one reflection to exclude from the agreement factor calculations. NOTE: use the rearranged indices here if the input indices are not those to be output
	6-10	KEXCL(I,2)	
	11-15	KEXCL(I,3)	

8. (I1,F3.0,2F4.0,F11.3,F10.3,I3,6F6.3,F8.5)

Reflection data here, on cards, if ICN=1.

9. (I1,F3.0,2F4.0,F11.3,F10.3,I3,6F6.3,F8.5)

Terminator reflection (a dummy with ISENT=1). Actually this record is a "Linus blanket" since an EOF(5) check can sense the end quite adequately.

Output

DATA Binary, suitable for least squares input. Compatible with LINUS, etc.

Each logical record contains:

ISENT	data list terminator (=0 for good datum, = 1 on dummy terminator record)
IHHH,IKKK,ILLL	Miller indices (h,k,ℓ)
FAV	Weighted average; F or F**2
WAV	Sigma of FAV (see Method)
ISF	Scale factor number (= input value (Card 6 above) for measured ref, = 99 for synthetic datum).
(ETEMP(K),K=1,7)	Components of normals (K=1,6), and $\bar{T}$(K=7), for absorption and extinction (see Program BNLABS).
ETEMP(8)	Sigma(FMEAN), included if user desires this information at a later date.
(PAD(I),I=1,18)	All = 0. Dummy fields for later use.

DATA terminated with a dummy reflection bearing ISENT = 1, followed by an ENDFILE.

TAPE3: BCD

Each logical record contains the same information as records on DATA, with the exception that the records are not padded with the 18 dummy words, and the intensities and sigmas have been scaled such that SF_{max} is .LE. 9999999. Scale factor applied is indicated. Also, if ETEMP(8) .GE. 999.9, it is set = 999.9. Formatted according to the following:

FØRMAT(I1,I3,2I4,F11.3,F10.3,I3,6F6.3,F8.5,F5.1)

Terminated identically as DATA.

Punch: To obtain punched output the user must write a small program which will read either of the above two output files extract the information he needs and transmit this to cards. *NOTE* the records of TAPE3 are each of 85 characters and so a simple copy to PUNCH will not work.

PRINTED: (on File OUTPUT) Title, cell constants, wavelength, and control integers. number of reflections read, and number of these accepted. Data search limits (user specified or program determined, and relative locations (in octal) of sorting arrays. Location of MHKL (number accepted) is the last location required by the program. This is checked internally, and in subsequent runs the requested FL should be rounded up to the nearest 1000K above this. The program does RFL down, in any case, to the proper location. (Necessary ECS field length noted for future reference).

Each reflection output: (Header lists FTERM, but input may be F or F**2). List of equivalent reflections, including individual intensities and sigmas, components of normals, $\bar{T}$, and the reflections position in the input list. (One or more asterisks denote reflections that have been rejected, based upon the users criteria).

Averaged data for DATA/TAPE3 is then listed: Miller indices, rearranged as per *SPACE*; weighted average intensity; sigma of average; scale factor number; sin(THETA); number of equivalent reflections followed by the number rejected; components of normals, $\bar{T}$ (averaged over all the contributors); sigma(FMEAN) and its fractional vaule, based on FMEAN.

The proper components of normals are output by the program, with the following exception: if the *SPACE* rearranged indices do not in fact appear in the equivalent reflections list, then there will not be a set of normal components which correspond to the orientation of the h,k,ℓ values to be written on DATA/TAPE3. In this case, AVSORT puts out the set of normals corresponding to the last reflection in the equivalence list. *NOTE* IF SYMMETRY EQUIVALENT REFLECTIONS ARE AVERAGED THEN THE RESULTING DATA SET WILL BE QUITE UNSATISFACTORY FOR THE DETERMINATION OF ANISOTROPIC EXTINCTION PARAMETERS AND THE COMPONENTS OF NORMALS WILL BECOME USELESS QUANTITIES. HOWEVER IN MOST CASES THE AVERAGED TBAR TERMS SHOULD REMAIN USEFUL FOR THE EVALUATION OF ISOTROPIC EXTINCTION.

If under certain conditions, all n of n equivalent reflections are rejected, the program recalculates FMEAN deleting that reflection which exhibits the worst (unweighted) agreement, and reexamines the equivalence list. Agreement factors are not affected, as rejected reflection are always included in the calculation of R and WR.

**** A series of 4 asterisks precedes the scale factor number to flag a reflection that has only two contributors, whose two intensities do not satisfy the acceptance criteria set by the user. The averaged data is output on DATA/TAPE3, the asterisks appear only on the printed output for reference purposes.

Agreement factors put out after end of data. Mostly self explanatory, except:

Number of reflections for least squares input is Number on DATA/TAPE3

Number of disparate Doubly Determined Reflections is number flagged with **** on printed output. The (h,k,ℓ) are tabulated.

SHORT FORM PRINTED OUTPUT: (on file SHORT1) This file contains summary information abstracted from the complete output described above. SHORT1 consists of lines containing 60 characters and is designed for printing on a teletype. The contents of SHORT1 are as follows:

1. Title, cell constants, wavelength, control integers.
2. Number of reflections read; data search limits and program storage requirements.
3. Listing of bad observations determined
   a. Disparate doubly determined reflections are flagged ****.
   b. Individual bad observations (for reflections with more than 2 observations) are flagged with two or three asterisks depending on which test was failed. In this case the mean F^2 is printed but not flagged.
4. Agreement factors and summary giving number of reflections as well as number rejected.

For a typical run processing 1300 reflections of which about 40 were rejected, SHØRT1 contained about 110 lines of output.

Replaceable Routines:

SUBROUTINE IMP

The version supplied is a general routine suitable for most input purposes. It reads BCD cards or file, or binary file as per the following coding:

```
      SUBROUTINE IMP(IDENT,FH,FK,FL,SF,WEIGHT,SCALEN,
     1E1,E2,E3,E4,E5,E6,E7,ICN)
      GOTO(1,4,5),ICN
    1 READ  2, IDENT,FH,FK,FL,SF,WEIGHT,SCALEN,E1,E2,E3,E4,E5,E6,E7
      IF(EOF(5))6,3
    2 FORMAT(I1,F3.0,2F4.0,F11.3,F10.3,I3,6F6.3,F8.5)
    3 RETURN
    4 READ(1,2) IDENT,FH,FK,FL,SF,WEIGHT,SCALEN,E1,E2,E3,E4,E5,E6,E7
      IF(EOF(1))6,3
    5 READ(1  ) IDENT,JH,JK,JL,SF,WEIGHT,SCALEN,E1,E2,E3,E4,E5,E6,E7
      IF(EOF(1))6,3
      FH=JH
      FK=JK
      FL=JL
    6 IDENT=1
      RETURN
      END
```

For other special purposes, *IMP* should be altered. Specifically, the rejection of reflections if desired, based upon any criteria, so that they will not appear in the input list. The only other way of rejecting reflections on input is via the sinθ limits above.

SUBROUTINE REJECT(FH,FK,FL,IREJ)

This subroutine is called after the generated indices have been checked against the sinθ limits but before the systematic absences (card 3) are interrogated to ensure that the index triple is indeed wanted. This routine will be most useful if the user wants to reject a specific triple or if he/she wants to have unmeasured reflections output but cannot specify all of the systematic absences appropriate within the tests supplied. The version supplied is a dummy. If IREJ=0 the index triple is accepted, rejection occurs if IREJ=1

SUBROUTINE SPACE

This subroutine applies the diffraction symmetry by transforming the indices into those desired. The routine supplied is a dummy version of the second procedure (see below) which applies only the identity transformation. If the diffraction symmetry is triclinic, monoclinic or orthorhombic then the first procedure will probably be the most useful and popular. The example of a replacement version for SPACE appropriate to a monoclinic pattern should clarify this first approach.

```
      SUBROUTINE SPACE(FH,FK,FL)

C     THIS VERSION APPLIES 2/M SYMMETRY AND ALWAYS RETURNS THE REFLECTION
C     IN THE +H,+K,+/-L QUADRANT

      FK = ABS(FK)
      IF(FH) 1,2,3
    1 FH = -FH
      FL = -FL
    3 RETURN
    2 FL = ABS(FL)
      GO TO 3
      END
```

For diffraction data obtained from crystals of high symmetry the logic involved in writing a special subroutine according to the above procedure can become exceedingly complex and so to avoid unnecessary brain strain a second procedure was developed.

In this method the two tasks , (i) index transformation and (ii) testing if the new triple is the one desired are separated. Reciprocal space symmetry matrices are provided via BLOCK DATA SYMOPS to SUBROUTINE SPACE and these are used to generate new index triples from the FH,FK,FL supplied. As each new triple is generated SUBROUTINE FORM is called to check for acceptibility. The user must program into FORM those restrictions he wishes to apply to the generated triples, for example in a trigonal situation (c unique) he may require that $\ell \geq 0$ and that $h \geq k \geq o$. Such conditions could be programmed as:

```
      SUBROUTINE FORM(IFORM,H)
      DIMENSION  H(3)
      IFORM = 0
      IF(H(3).LT.0.0)  GO TO 1
      IF(H(2).LT.0.0)  GO TO 1
      IF(H(1).LT.H(2)) GO TO 1
      IFORM = 1
    1 RETURN
      END
```

Note that IFORM=1 implies acceptance whereas IFORM=0 instructs the program to apply another symmetry transformation and try again.

If the program is unable to satisfy the users requirements in this regard then a message is produced and the original indices input are returned to the main program.

The BLOCK DATA SYMOPS subprogram must contain the number of symmetry transformations to be applied (NEQV $\leq$ 24) and twenty-four 3x3 symmetry matrices, only the first NEQV of which need be non zero. The dummy version supplied is listed below.

```
      BLOCK DATA SYMOPS
      COMMON /SYMEQV/ NEQV, S(3,3,24)
      DATA NEQV/  1/
      DATA((S(I,J, 1),I=1,3),J=1,3)/ 1., 0., 0., 0., 1., 0., 0., 0., 1./
      DATA((S(I,J, 2),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 3),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 4),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 5),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 6),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 7),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 8),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J, 9),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,10),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,11),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,12),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,13),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,14),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,15),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,16),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,17),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,18),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,19),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,20),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,21),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,22),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,23),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      DATA((S(I,J,24),I=1,3),J=1,3)/ 0., 0., 0., 0., 0., 0., 0., 0., 0./
      END
```

Lest the user despair at this stage, be aware that a separate program (INVTRP) has been written which will produce, from user-input real-space symmetry matrices, a complete card deck for the BLOCK DATA SYMOPS subprogram appropriate to his/her reciprocal space symmetry.

Example: 4637 reflections have been processed on the 6600 under SCOPE 3.4. They required 77K of ECS. The inclusive range of (h,k,ℓ) was

(0,-15,-11) to (14,13,10)

The time required was 60_{10} sec. This program will run in considerably less time on the 7600 under SCOPE 2.1 without any modification.

Program Termination:

STOP 777 in day file for normal program exit.

Method: An input reflection is tested for inclusion in the sinθ range, and rejected if outside the range. Accepted data are then stored in arrays MHKL (packed indices), KEX1 and KEX2 (packed components of normals), SF (intensity), WEIGHT (sigma), and EX ($\bar{T}$). All arrays other than MHKL are written onto ECS almost immediately.

MHKL is an array which contains 3 packed integer variables per word. Two of these integer variables are themselves packed quantities and each contain 3 reflection indices. Each word in MHKL then contains 7 items. The words in MHKL contain the following packed information.

60 bits	=	20 characters, arranged as follows: (highest order bits--------lowest order bits)
MHKL(N+1)	=	0 01377 2001062 2001062 X N 'MHKL' HKL
X	=	bits 57-59: bit 59 is the sign and is not affected by right shifts, consequently it must never be set.
N	=	reference index, i.e., this labels the Nth reflection accepted. Necessary as a label for sequencing other arrays. Nth reflection is stored in location (N+1) since routine *QIKS* uses location (1) for sorting.
HKL	=	the packed indices as read in, for the Nth reflection accepted. Routine *PACK* converts (h,k,ℓ) to an integer variable, HKL: $2001062_8 = 524850_{10}$ = (2,-2,0)
'MHKL'	=	the Nth (h,k,ℓ) indices as rearranged by routine *SPACE*. Temporarily stored in location MHKL(N+1) until the variables N and HKL are computed and added, in their proper bit assignments. In the example above, the (h,k,ℓ) have not been rearranged.

*****MHKL is currently dimensioned for 25000 (= 24999 reflections). The maximum number of reflections is not determined by the size of N (= 377777_8 = 131071_{10}), but by the number of bits available for HKL and MHKL. This is a direct function of how routine *PACKT* packs the indices. Currently, *PACKT* computes an integer

$$505050_{10}$$

and adds to it H*10000 + K*100 + ℓ, i.e.,

```
  505050
+  H0000
+    K00
+      L
-------
=   HKL
```

Consequently, the limits of the program are defined by the way *PACKT* packs the indices, not by the size of MHKL. This must be taken into consideration if more than 24999 pieces of data are to be processed in one run. The permissible ranges of (h,k,ℓ) are

(-50,-50,-50) to (49,49,49) inclusive.

See Example, also.

If data beyond any of these individual h,k, or ℓ limits are necessary, substantial reprogramming must be done. If greater than 24999 pieces of data, all within these limits, are desired, simple increase of the dimensions of MHKL in all pertinent routines is necessary and sufficient. If more than 300 observations of any one reflection (and its equivalents) exist, then the dimensions of the following arrays must be altered, as must the EQUIVALENCE statement in which they appear:

FTEMP, WTEMP, SIGMA, HTEMP, K1TEMP, K2TEMP, and EXTEMP

The MHKL array is sorted by *QIKS* in ascending order on the *SPACE* rearranged indices; HKL and N are carried along with the sorting process. (*COMPARE* and *MOVE* are used by *QIKS*, *COMPARE* abstracts from MHKL the proper bit content for sorting). The remaining arrays in ECS are then rearranged according to the new order specified in MHKL, and rewritten onto ECS.

The program then generates such reflection triplet beginning at the low limit on each of the three indices and ascertains if its value is in the array MHKL. If the program generated triplet is not equal to the next value of MHKL to be tested, but is less than this value, it is treated as unmeasured. (If its value is less than the next value of MHKL, there are no observations of the particular (h,k,ℓ), since MHKL has been sorted). The unmeasured reflections may or may not be output on DATA/TAPE3, depending upon the value of IUN. If the (h,k,ℓ) is equal to the next value of MHKL to be tested, all equivalent reflections are removed (moving right up MHKL) and treated as below. If the (h,k,ℓ) is larger than the next value of MHKL,

then the program moves up MHKL until it finds a value equal to, or greater than the (h,k,ℓ), and treats it as above. The latter case may occur depending upon how the user employs the routines *SPACE* and *REJECT*. The process continues until all values between the index limits have been checked.

The averages are computed as follows:

FAV = (∑(1/SIGMA**2) * F) / (1/∑SIGMA**2)

WAV = 1/SQRT(∑(1/SIGMA**2))

AVF = ∑F (all reflections, accepted or rejected: used for agreement factors)

ETEMP(8) = SQRT(1/(n-1) * ∑(ABS $(\bar{F}-F_n)^2$)

Although the program tests on the ETEMP(8) calculated above, this is converted to the estimated standard deviation of the mean by dividing by SQRT(n), i.e.,

ETEMP(8) = ETEMP(8)/SQRT(n)

This value is output as SIG(FMEAN).

Four agreement indices are provided by the program. These are computed from ALL measurements of the multiply determined reflections except those EXPLICITLY EXCLUDED BY THE USER using the NEXCL and KEXCL options described on page 4.

In the following definitions Wi and Fi are the weight $(1/\sigma_i^2)$ and value associated with the ith measurement. Assume that the index j runs from 1 to N over all of the multiply determined reflections for each of which there exist a variable n_j $(n_j \geq 2)$ number of measurements.

The index i ranges from 1 to n_j and specifies a contributor to the mean. The simple mean is denoted $\bar{F}_j$ and the weighted mean by $\hat{F}_j$.

Then

$$R_1 = \frac{\sum_{j=1}^{N} \frac{1}{n_j} \sum_{i=1}^{n_j} \left| F_{i,j} - \bar{F}_j \right|}{\sum_{j=i}^{N} \left| \bar{F}_j \right|}$$

$$R_2 = \frac{\sum_{j=1}^{N} \frac{1}{n_j} \sum_{i=1}^{n_j} W_{ij} \left| F_{ij} - \hat{F}_j \right|}{\sum_{j=1}^{N} \left| \hat{F}_j \right|}$$

$$R_3 = \frac{\sum_{j=1}^{N} \sum_{i=1}^{n_j} |F_{i,j} - \bar{F}_j|}{\sum_{j=1}^{N} |n_j . \bar{F}_j|}$$

$$R_4 = \frac{\sum_{j=1}^{N} \sum_{i=1}^{n_j} W_{ij} |F_{i,j} - \hat{F}|}{\sum_{j=1}^{N} n_j . \hat{W}_j . \hat{F}_j}$$

where $\hat{W}_j = \sum_{i=1}^{n_j} W_{i,j}$

Brookhaven Crystallographic Computer Program Writeup

PRØGRAM BNLABS(INPUT,ØUTPUT,PUNCH,TAPE2,TAPE3,TAPE4,TAPE5=INPUT,TAPE7=PUNCH)

Purpose: This is the second stage in processing of x-ray or neutron four-circle diffractometer data. Lorentz-polarization factors are applied, absorption corrections are made, and the necessary quantities for making extinction corrections in the Zachariasen approximation are calculated (Zachariasen, Acta Cryst. 23, 558 (1967); Coppens and Hamilton, Acta Cryst. A26, 71 (1970)). For details on the absorption correction see Coppens et al. (Acta Cryst. 18, 1035 (1965)). Input data is assumed to come from PRØCK (HFBR and Picker data).

BNLABS SUPERSEDES PRØGRAM DATAPH

This program uses the true setting angles in the calculation of transmission factors, mean path lengths, and components of vectors for anisotropic extinction. The true angles are read from cards or tape produced by PRØCK (see new writeup).

The input of true angles guarantees correct processing for reflections collected in any setting. If the true setting angles are not available and must be generated from the orientation matrix the angle calculation option will give setting angles in the hemisphere defined by $-90^{\circ} \leqslant \chi(\text{true}) \leqslant 90^{\circ}$. These angles will be modified by the user supplied ω(true) values (usually zero) but will nevertheless be incorrect for reflections collected in the upper hemisphere. This implies that the components of normals, transmission factor, etc. will be wrong for the reflections which were collected with $|\chi| > 90^{\circ}$.

Field Length: $(41000)_8 + (4*N_1*N_2*N_3)_8$

where N_1, N_2 and N_3 are the number of Gaussian grid points.

Time Required: Two examples may serve as a guide. These examples were run on a CDC 6600 under the old BNL SCØPE operating system.

1) No absorption: 1302 reflections in 18.3 sec CP time.
2) 512 point grid and 8 planes: 2185 reflections in 540 sec CP time. Run as an A job.

Files Required: TAPE3 input, optional (From PRØCK)
TAPE4 output, optional (BINARY)
TAPE2 output, optional (BCD)

Input:

Card 1. FØRMAT(1X,79H) Title. Punch in columns 2-80.

Card 2. FØRMAT(7F9.6) Reciprocal Cell Constants, Monochromator 2θ
$a^*, b^*, c^*, \cos\alpha^*, \cos\beta^*, \cos\gamma^*, 2\theta_m$ (may omit $2\theta_m$ for neutron data)

Card 3. FØRMAT(9F8.0) $((U^B(I,J),J=1,3),I=1,3)$ where $U_{ij}{}^B$ is inverted normalized U matrix defined by Coppens and Bednowitz and is printed out by ØRIENT or the NEXDAS command LS at the HFBR. If the transformation matrix U is defined as in Hamilton's International Tables article:

$$A^* \equiv UA_o$$

where A^* are the reciprocal cell coordinates, and A_o is an orthogonal system fixed in the goniometer head, then the U^B matrix here is obtained from U by dividing the rows of U by a^*, b^*, c^* respectively and taking the transpose. See appendix. If absorption and extinction corrections are undesired, this matrix is irrelevant. Columns of the U matrix should be normalized to unity. The program prints the matrix out as input and after normalization.

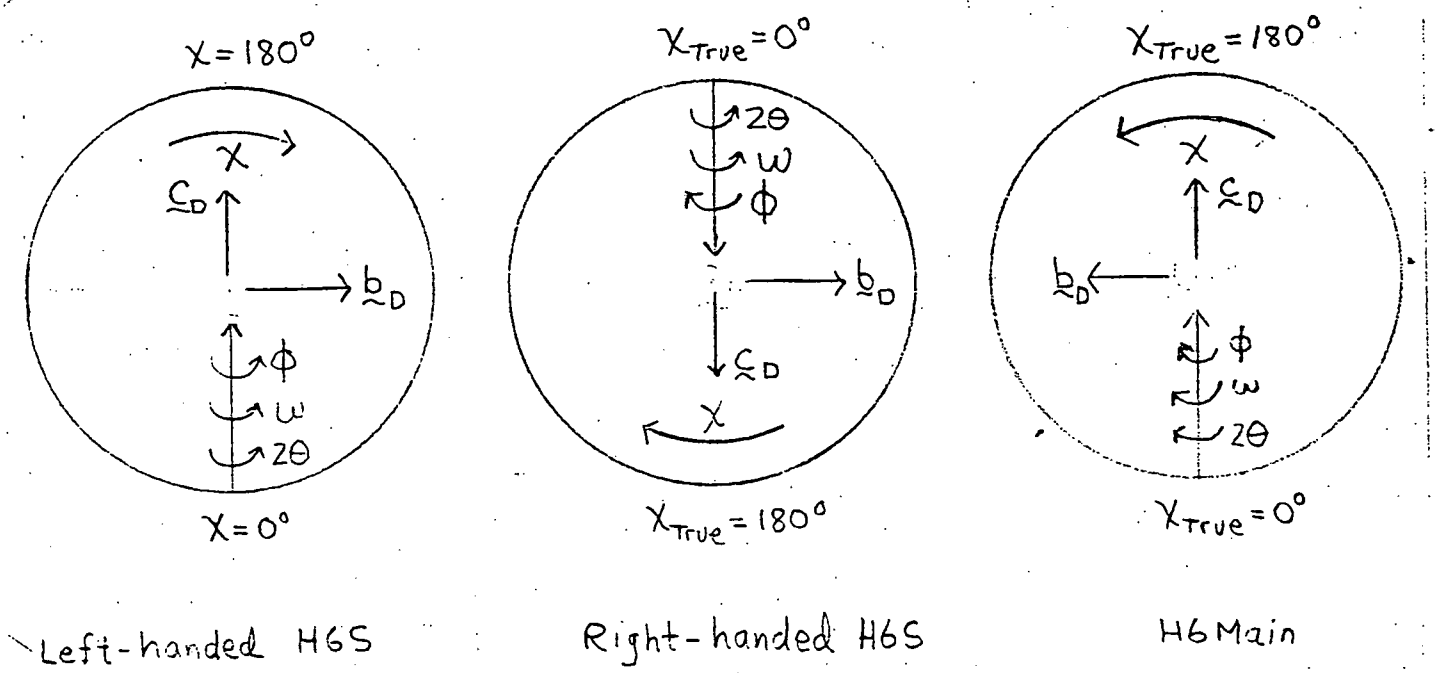
Note (which can be understood by BNL users only): To process data from XRAY or MAIN, the orientation matrix input to BNLABS should be exactly as typed out by NEXDAS at the HFBR. The parity (all negative for both machines) and mechanical zeroes used in the data collection programs should be input to PRØCK, which will produce true values of ω, χ and ϕ.

The detector on the H6S neutron diffractometer moves in the opposite sense from that on the main machine or the Picker. The diffractometer coordinate system (a_D, b_D, c_D) with which we work during data collection is thus left-handed for this diffractometer (see below). We also find it convenient to call χ 0° when the goniometer head is at the bottom of the circle (true $\chi \approx 180^o$) with respect to the sense of 2θ for this machine. In order to obtain true setting angles referred to a right-handed diffractometer coordinate system, and to maintain consistency between the three machines, the following procedure should be observed while processing data from SATT using PRØCK and BNLABS.

(1) add 180° to χ_o used in data collection and input this value as CHIZERØ in PRØCK. Insert ω_o and ϕ_o used in data collection without any change.

(2) reverse the parity of phi, so the parity input to PRØCK becomes $-\omega$, $+\chi$, $+\phi$, rather than the $-\omega$, $+\chi$, $-\phi$ used by NEXDAS for the satellite machine

(3) The U matrix input to BNLABS should have the signs of the second and third rows reversed from the way they are typed out of H6S3.



Left-handed H6S Right-handed H6S H6 Main

Card 4. FORMAT(16I5) Control Integers (ICN(I),I=1,16)

ICN(1) Cols 1-5 = 0 no absorption correction.
= 1 absorption correction is applied.

(2) Cols 6-10 = 0 no quantities are calculated for extinction.
= +1 Quantities necessary for extinction correction in LINUS (the Brookhaven least-squares program) are calculated.
= -1 Vector components but not $\bar{T}$ are calculated for extinction.

(3) Cols 11-15 non-zero. A subroutine SCALE is called which may be used to scale data relative to standards collected during data collection procedure.

(4) Cols 16-20 = 0 use input setting angles.
= 1 calculate setting angles from matrix (above) and value of omega supplied with each reflection.

(5) Cols 21-25 = -1 Apply neither Lorentz nor polarization corrections.
= 0 Apply Lorentz and polarization corrections - for the X-ray case.
= 1 Apply Lorentz correction only - for the neutron case.

(6) Cols 26-30 Determine status of BCD output.
= 0 no punched card output of reflections, no BCD tape.
= 1 for punched card output in format suitable for input to LINUS or AVSORT.
= 2 for output on BCD TAPE2 in format suitable for input to LINUS or AVSORT.

(7) Cols 31-35 Determines status of binary TAPE4 for least-squares input.
= 0 for no TAPE4 output.
> 0 for new TAPE4 output.

(8) Cols 36-40 0 for card input as described below. } check 66-70
1 for input from TAPE3 as described below. } this card

(9) Cols 41-45 = 0 normally.
≠ 0 for setting angles check. If ICN(9) is not zero this card should be followed by ICN(9) cards of format (3F3.0,F9.3) with h,k,ℓ and true value of omega. The program will calculate and print the setting angles for these reflections.

(10) Cols 46-50 No longer active.

(11) Cols 51-55 0 full information printed out.
1 abbreviated printed output.
2 messages only output after each 10 reflections processed.

(12) Cols 56-60 No longer active.

(13) Cols 61-65 No longer active.

(14) Cols 66-70 = 0 standard input format.
> 0 long records containing scale in F10.3 and sequence number at end. (see the PRØCK write-up)

The inactive fields on card 4 and ICN(I), I = 15-16 are read in (as integers) and are available to the user-supplied subroutines for whatever purpose.

Card 5. Optional FØRMAT(3F3.0,F9.3) cards for angle check. Refer to ICN(9) above. These cards contain h,k,ℓ and ω.

Card 6. Optional - supply only if ICN(1) or ICN(2) is +1. FORMAT(4I5) Specifications for grid for absorption or extinction correction. A Gaussian integration formula is used. The first three fields define the number of grid points in various directions. The product of these three must be less than the second dimension of GRID in the main program. The version of program available is compiled for this dimension equal to 5000.

Cols 1-5 Number of Gaussian grid points along a. } must be even numbers
Cols 6-10 Number of Gaussian grid points along b. } in the range 2-16,
Cols 11-15 Number of Gaussian grid points along c. } or 24, or 32.

Cols 16-20 Number of boundary planes

Card 7. Optional (supply if Card 6 supplied). FORMAT(4F10.4)
One card for each boundary plane. These are given in terms of the Miller indices of crystallographic planes and the perpendicular distances in cm of these planes from an arbitrary origin within or on the surface of the crystal.

Cols 1-10 h

Cols 11-20 k

Cols 21-30 ℓ

Cols 31-40 distance in CENTIMETERS *NOTE* CENTIMETERS NOT mm.

Card 8. FORMAT(I5,7F10.5). Reflection batch card.

Cols 1-5 IQ Scale factor number IQ will be punched on output cards if NSCALE is set to 1 in IMP; for other values of NSCALE the scale factor number is taken equal to NSCALE.

Cols 6-15 Wavelength of radiation in Å.

Cols 16-25 c_1

Cols 26-35 c_2

the program will calculate $\sigma^2(I-B)$ as $(I+B) + c_1{}^2(I-B)^2 + c_2{}^2(I_{corrected}-I)^2$

The three terms represent the statistical error, a proportional error and the uncertainty in the absorption correction. I (WCH) recommend $C_1=C_2=0$ and change weights in the least-squares program.

The term c_1 is often called the "ignorance factor" and is designed to allow for unknown factors affecting the experimental stability. In many X-ray situations the dominant contributor to c_1 is the uncertainty in the scale factor which accounts for the decomposition of the crystal. This scale factor is usually computed from the monitor reflections and its uncertainty should be obtainable from the spread of these data. A recent paper (McCandlish, Stout and Andrews, Acta Cryst. A31, part 2, 245-249 (1975). bears on this problem and should be consulted. Although WCH's suggestion above undoubtedly has merit it seems that a better procedure would be to perform some analysis of the monitor reflections and to modify the variance accordingly. Unfortunately the small amount of programming necessary to implement this approach has not been included in the current version of the program. Refer to program CORDAT if this is a problem. The c_2 term probably should be included at this stage because after this program has been run only the $I_{corrected}$ term is available to the user, who cannot then incorporate $I_{corr}-I_{uncorr}$ into his/her calculations.

Cols 36-45 μ, absorption coefficient in reciprocal cm.

Cols 46-55 Scale factor by which F^2 is multiplied. Must not be zero. 1.0 is often appropriate.

Card 9. FORMAT(6I3) standard reflection indices. This card supplied only if subroutine SCALE is called as specified on Card 4 in field 3.

H1, K1, L1, H2, K2, L2

Card 10. Reflection data cards as called for by subroutine IMP.

For input from PRØCK the routine is called CALL IMP(FH,FK,FL,S,B, SCB,OM,PHI,CHI,SLO,SLB,OBSFI,BACFK,IDENT,NSCALE,ICN,JSEQ)

A call is made to this routine to read each reflection in turn. The first 14 arguments must be returned by the subroutine to the calling program. ICN(16) are the control integers which may be used by the programmer. Only the ones described under Card 4 (above) have special meaning in the program, and the others provide some flexibility in data manipulation. NSCALE is a scale factor number which is simply transferred to the output. IDENT should be returned as 0 if this is a reflection.

IF(IDENT .EQ. 0)	This is a reflection.
IF(IDENT .EQ. 1)	New cards 8 and 9 plus new calls to IMP will be made.
IF(IDENT .EQ. 2)	Run is terminated.
IF(IDENT .EQ. 3)	A complete new run with new title, etc. is started.
IF(IDENT .GT. 3)	New Card 9 plus new calls to IMP will be made.

The routine supplied requires cards in the following format if ICN(8)=0. IF ICN(8)=1, BCD TAPE3 input in the same format is required. FORMAT (3F3.0,2F10.1,F6.3,3F7.2,2F3.0,2F8.0,I2)--but refer to ICN(14) above and to the PRØCK writeup for the case of LONG input records.

Cols 1-3	FH = h	
Cols 4-6	FK = k	
Cols 7-9	FL = ℓ	
Cols 10-19	S	total count over those steps of the scan deemed to comprise the peak.
Cols 20-29	B	total count over those steps considered to be background.
Cols 30-35	SCN	scale factor applied to this reflection (if left blank, SCB is set = 1).
Cols 36-42	OM	(true) at which reflection was collected.
Cols 43-49	PHI	(true).
Cols 50-56	CHI	(true).
Cols 57-59	SLO	number of points in peak.
Cols 60-62	SLB	number of points in background.
Cols 63-70	ØBSFI	corrected number of counts for statistics if smoothing or scaling was done in PRØCK.
Cols 71-78	BACFK	corrected number of counts in background.
Cols 79-80	IDENT=2	for data termination (cards only) if TAPE3 input is used, EØF for data termination.
	JSEQ	For LONG input records see the PRØCK writeup.

Replaceable subroutines

IMP as defined above may be changed to vary input format.

SUBROUTINE SCALE(IH,IK,IL,ISIG,M,NSCALE,NREJ,JM,H1,K1,L1,H2,K2,L2,TODAY,JSEQ)
This routine is called shortly after IMP for every reflection.

IH,IK,IL are Miller indices of reflection.
H1,K1,L1,H2,K2,L2 are integer Miller indices of the monitor reflections.
ISIG is the net peak count. M is the integrated background count.
NSCALE is the scale factor number as supplied by IMP.
NREJ may be returned not equal to 0, and reflection will be rejected.
JM is serial counter of the reflections as they are read in.
TODAY is a scale factor--initially 1.0--which may be calculated by this routine and multiplies the scale factor on the Input cards and that specified on the batch card.

The routine supplied does the following:

1) Sets NSCALE = 1.

2) If the two standard reflections have occurred together in either order after the first such occurrence, the old scale factor is multiplied by

$$\frac{\text{Old Total net peak count for the two reflections}}{\text{New Total net peak count for the two reflections}}$$

Initial scale factor is 1.0.

3) If this factor lies between 0.98 and 1.02, the routine returns with SCLA equal to the old scale factor. If it is outside this range, the routine returns with SCLA equal to the new scale factor.

For various reasons the user may consider the stepped scale function (immediately above) unsatisfactory and prefer to write his/her own routine which will provide a smoothly varying scale factor as a function of reflection sequence number. It is for just this purpose that JSEQ, which is the true RECF (previously MSCS) sequence number associated with the reflection. Note that JSEQ is only available if LONG records were output by PROCK and read into this program.

Output:

Binary TAPE4, or cards or BCD TAPE2 with FORMAT(3I4,F11.3,F10.3,I3,6F6.3,F8.5,F5.1)
Following data is included, one record for each reflection.

JDENT = 0 normally.
= 1 on dummy record following last reflection. This dummy record is NOT output to PUNCH.

H
K [Integers]
L

FSQ = [S-(SLØ/SLB)]*B*)1/Lp)*(1/ABS)*(Scale factor from subroutine SCALE)*(scale factor from reflection batch card)

A

σ^2(FSQ) = [ØBSFI+((SLØ/SLB)**2)*BACFK]*(correction factors and scale factors as for FSQ)

Non-Poisson error can if desired be added in by supplying proper information on Card 8. WCH does not like to do this here.

JSCL scale factor number (integer)

XN(1), XN(2), XN(3) — components parallel to a, b, and c in Å of the unit vector normal to the plane containing the incident and diffracted beams.

XNSØ(2), XNSØ(2), XNSØ(3) — components of unit vector normal to incident beam in the plane of the incident and diffracted beams.

TBAR mean path length for this reflection--weighted by absorption.

(The last seven quantities may be used in calculation of anisotropic extinction corrections (Coppens and Hamilton, 1968.)

PAD A 5 character pad to retain compatibility with AVSORT as input to FLINUS. This pad is NOT output on the records to PUNCH.

Appendix

Definition of the U^β matrix

The U^β matrix relates the reciprocal lattice axes a*, b* and c* to the orthogonal right-handed goniometer head axes X, Y and Z.

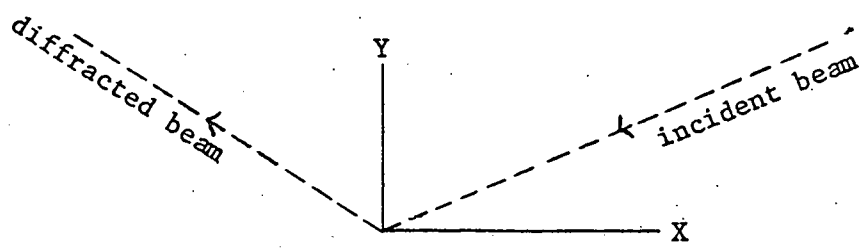
At zero values of the setting angles ϕ, χ and ω the axes are defined as follows: Y lies in the plane of the incident and diffracted beam and in the plane of the χ circle in a direction such that the incident beam arrives at the origin (crystal) from the positive x, positive y direction. X is paralled to the χ axis and therefore bisects the angle between the incident and diffracted beams (see figure). Z is parallel to the ϕ axis, such that the coordinate system is right handed.

If X, Y and Z are unit vectors parallel to the goniometer head axes X, Y and Z, U is defined by:

$$(\underline{X},\underline{Y},\underline{Z})\ U^\beta = \left(\frac{\underline{a}^*}{|a^*|}, \frac{\underline{b}^*}{|b^*|}, \frac{\underline{c}^*}{|c^*|} \right)$$

Therefore:

$$U^\beta = \begin{pmatrix} \cos(a^*,X) & \cos(b^*,X) & \cos(c^*,X) \\ \cos(a^*,Y) & \cos(b^*,Y) & \cos(c^*,Y) \\ \cos(a^*,Z) & \cos(b^*,Z) & \cos(c^*,Z) \end{pmatrix}$$



Note carefully that this U matrix "U_B" is related to Hamilton's U matrix U_H by the transformation

$$U_H(1,J) = a^* \; U_B(J,1)$$

$$U_H(2,J) = b^* \; U_B(J,2)$$

$$U_H(3,J) = c^* \; U_B(J,3)$$

Hamilton's U_H is used in GØNØ9 and in volume IV of the International Tables for Crystallography.

CAD4 - 6/22/76
AUTHOR: M. GRESS

BNL CRYSTALLOGRAPHIC PROGRAM

```
PROGRAM CAD4(INPUT,OUTPUT,TAPE1,TAPE2,TAPE3,TAPE4,TAPE5,TAPE6,
TAPE7,TAPE8,TAPE9,TAPE10,TAPE16,TAPE17=OUTPUT)
```

THIS DATA REDUCTION PROGRAM FOR THE CAD-4 DIFFRACTOMETER IS A MODIFICATION OF THE DATA REDUCTION PROGRAM SUPPLIED BY ENRAF-NONIUS. THE OUTPUT IS EITHER RAW INTENSITIES FOR ABSOR OR FSQ'S FOR AVSORT OR FLINUS.

INPUT CARD 1
FORMAT (5I2,3F10.6)

```
IFIL  = NUMBER OF INPUT DATA TAPES
IFORM = 0/1  WRITE OUTPUT DATA TAPE16 SUITABLE FOR ABSOR
        (ABSORPTION CORRECTION)/AVSORT OR FLINUS
ITAP  = 0/1  DO NOT/DO WRITE DIFFRACTOMETER RAW DATA ON
        TAPE17
NB    = NUMBER OF BACKGROUND POINTS AT EACH END OF THE
        SCAN (ZERO OR BLANK IMPLIES NB=16)
ISKIP = NUMBER OF SECTIONS OF RECORDS TO SKIP (CARDS 2)
        LIMIT 99
ATNN  = ATTENUATION FACTOR
FLAMB = WAVELENGTH
TTMON = TWO THETA FOR MONOCHROMATOR (NORMALLY 26.6 FOR
        COPPER OR 12.2 FOR MOLYBDENUM; ZERO OR BLANK
        IMPLIES NO MONOCHROMATOR WAS USED)
```

INPUT CARDS 2 (OPTIONAL)
FORMAT (2I10)
ISKIP1,ISKIP2

ONE CARD FOR EACH SECTION OF REFLECTIONS TO SKIP (I.E. FOR EACH SECTION, ISKIP1 IS THE FIRST REFLECTION TO SKIP AND ISKIP2 IS THE LAST)

OUTPUT FILES

TAPE16 FOR ABSOR
IH,IK,IL,OBS2,BAK2,SCB,OM,PHI,CHI,ISL,ISB,OBS2,BAK2,ID,NR1
FORMAT (3I3,2F10.1,F10.3,3F7.2,2I3,2F8.0,I2,I6)

TAPE16 FOR AVSORT OR FLINUS
JEND,IH,IK,IL,FSQ,SIGI,JSCL,EXT(7)
FORMAT (I1,I3,2I4,F11.3,F10.3,I3,6F6.3,F8.5)

TAPE17
IH,IK,IL,DATCOLCODES,PSI,NPI,IBL,IPK,IBR,CI,SIGCI,THETA,
PHI,OMEGA,CHI,SCAN,SCANTM,NR1,DSCALE
FORMAT (3I4,4X,A6,F7.2,I4,I6,I7,I6,F10.2,F9.2,F8.3,4F9.3,
F6.1,I7,F7.3)

BNL Crystallographic Computer Program Writeup

CØMPARE SCØPE 3.4/2.1

PRØGRAM CØMPARE(INPUT,ØUTPUT,TAPE1,PLØT,TAPE11=PLØT,TAPE6=ØUTPUT,
FØUR,TAPE2=FØUR)

Purpose:

Carries out statistical comparisons, including χ^2 tests and preparation of normal probability plots, for two sets of atomic parameters or between two or more structure factor data sets. The program may also be used to perform comparisons between all pair-wise combinations of up to 7 sets of quantities of a general nature.

Operating characteristics:

Field length (51K)
Time 5 seconds for 200 pairs of atomic parameters on the CDC 7600.

Limitations:

A. A maximum of 450 pairs of atomic parameters may be accommodated.
B. Up to 2248 pairs of structure factors may be compared.
C. Isotropic temperature factors are currently not permitted.
D. For multiple comparisons up to 7 sets of up to 100 parameters may be used.

Input:

Card 1 FØRMAT(8A10)

cols	1-10	Identification for first data set.
	11-20	Identification for second data set.
	21-60	Will appear on plots.
	61-80	Will appear on printout but not on plots.

Card 2 FØRMAT(8I10)

cols	1-10	Number of parameters. } In each set of crystallographic parameters.
	11-20	Number of atoms. } In each set of crystallographic parameters.
	21-30	Number of unrefined position parameters.
	31-40	Number of unrefined thermal parameters.
	41-50	= 0 no normal probability plot. = 1 printer plot only. = 2 printer plot and CALCØMP plot.
	51-60	= 0 comparison of structural parameters for two sets of crystallographic results. = 1 structure factor or other general comparison between two or more parameter sets.

Cards 3 If col. 60 of card 2 above contains "1" skip this paragraph and see "B" below.

A. (for cc 60 of Card 2 = 0) The user has opted for a comparison of two sets of crystallographic parameters (fractional coordinates and anisotropic thermal vibration terms). The parameters of each set are supplied in independent decks each of which is an FLINUS style parameter deck (without the leading scale and overall B cards or the trailing extinction term(s) card). Each parameter deck must be preceded by one card containing the unit cell parameters if conversion of the β_{ij}'s to U_{ij}'s is desired. If no conversion of the thermal motion terms is required (U's supplied) then this preceding card should be blank. The set-up of these cards is:

(i) Cell card for parameter set 1 (real or reciprocal, degrees or cosines in 6F9.6; use a blank if U_{ij}'s are supplied).

(iia) Name, x,y,z for atom 1 of parameter set 1 (A6,21X,3F9.6)

(iib) Name, $\sigma_x,\sigma_y,\sigma_z$ for atom 1 of parameter set 1 (27X,3F9.6)

(iic) $\beta_{11},\beta_{22},\beta_{33},\beta_{12},\beta_{13},\beta_{23}$ for atom 1 of parameter set 1 (6F9.6)

(iid) $\sigma_{\beta_{11}},\sigma_{\beta_{22}},\sigma_{\beta_{33}},\sigma_{\beta_{12}},\sigma_{\beta_{13}},\sigma_{\beta_{23}}$ for atom 1 of parameter set 1 (6F9.6)

Cards (iia) - (iid) repeat for NATØM groups.

(iii) Cell card for parameter set 2.

(iva) Name, fractional coordinates

(ivb) Coordinates, standard deviations

(ivc) β_{11}, etc.

(ivd) Temperature parameters standard deviations

Comments as above apply.

For the user who does not like this procedure the input routines GETP and READP may be modified.

Now read under Card 4 below.

B. (for cc 60 of card 2 = 1) A choice between a comparison of two sets of crystallographic structure factors or multiple two-way comparisons between all pairs of up to 7 sets of generalized parameters still exists. If a single comparison of two sets of structure factors is desired, skip this section and read C below.

The various parameter sets (up to 7 sets of up to 100 parameters each) are supplied separately: a parameter identifier, the parameter and its standard deviation on each of NPAR cards. Each set of parameters is preceded by a card containing an identifier for the set and the input deck is preceded by card bearing the number of sets and the number of parameters in each.

The setup is

(i) (2I10)

cols	1-10	NSET	No. of sets of parameters to CØMPARE
	11-20	NPAR	No. of parameters in each set

(ii) (A10) repeats NSET times

cols	1-10	Title for J'th parameter set	TITRE(J)

(iii) (A10,2F10.4) repeats NPAR times

cols	1-10	NAME(I,J)	parameter identifier
	11-20	F(I,J)	parameter value
	21-30	S(I,J)	sigma value

CØMPARE will use the standard SFIN routine to carry out NSET(NSET-1)/2 pair-wise comparisons of NSET sets of parameters.

C. A simple comparison of structure factors is desired. To exercise this option supply two blank cards here and use the alternate SFIN routine listed below instead of that supplied by default.

```
      SUBROUTINE SFIN(X,ID,NF,NPAR,KSET,LSET)
      COMMON TAR(3600),XAR(151),BAR(301),IDX(151),IDB(301)
     1,TITLE(8),IC(8),TOR(63)
      COMMON NDF(9)
      COMMON TITRE(7),NAME(100,7),F(100,7),S(100,7)
      DIMENSION X(2250),ID(2250)
      REAL ID
      DO 1 I=1,2248
      READ (2)IH,IK,IL,TWO,FO,FC,CO,SI,DEL,SIGMA
      IF(EOF(2))2,3
3     ENCODE(9,4,ID(I))IH,IK,IL
4     FORMAT(3I3)
1     X(I)=DEL/SIGMA
      NF=2248
      RETURN
2     NF=I-1
      RETURN
      END
```

Note that this will process only the first 2248 structure factors, which is currently the limit. A different SFIN routine will be needed if file FØUR contains other than structure factor data in the standard form. Array X contains Δ/σ values and array ID contains coded identifiers for these values. SFIN is called if and only if col 60 is non-zero.

Card 4 Blank if reinitiation of the program starting with Card 1 is desired. Otherwise a 1 in column 1 for final termination.

FILES (1) If CALCØMP plots are requested, the data for the plot are written on file PLØT.

(2) TAPE1 (BCD) will have the same statistical information as appears on the output file in a form appropriate for direct reproduction for publication.

(3) FØUR may contain structure factor or other data.

ØUTPUT:

The output consists of a tabulation of Δ/σ for each parameter

$$x,\ \sigma(x_1),\ x_2,\ \sigma(x_2),\ x_1-x_2\ \ \sigma(x_1-x_2),\ \frac{x_1-x_2}{\sigma(x_1-x_2)}$$

Information for χ^2 tests for all parameters
Contrast tests on mean parameters

Normal probability plots for positional and thermal parameters or for structure factors.

For understanding of contrasts, see Hamilton, Acta Cryst. A25, 194 (1969).

The principal crystallographic reference for Normal Probability Plot Analysis is: Abrahams and Keve, Acta Cryst. A27, 157-165 (1971).

Note This program will always attempt to initialize the PLOT package and so the CALCMP routines must be supplied.

Brookhaven Crystallographic Computer Program

COORD

Field Length: <20K Time: <5 sec

Purpose:

This program, which is a revision and correction of an earlier program of the same name, is designed to produce a publishable listing of atomic parameters. Either cards or files produced by FREDFUN may be used to input the atomic parameters. Standard deviations, if supplied, are output with the parameters.

Input Quantities:

Card 1 TITLE FØRMAT (10A8)

Card 2 Cell parameters (real or reciprocal)
FØRMAT (6F9.6)

Card 3 Control integers FØRMAT (8I3)

cc 1 - 3	NATØM		The number of atoms. (Maximum is 62)
4 - 6	NANISØ		The number of atoms with anisotropic thermal parameters. It is assumed that these all occur in the input stream before any isotropic atoms are encountered.
7 - 9	IFØRM	= 0	Transform the input β's to U's for the anisotropic atoms.
		= 1	Transform the input U's to β's.
		= 2	No transformation of the parameters for anisotropic vibration.
			See Note 4.
10 - 12	IPUNCH	= 0	No punched output.
		= 1	Punch x,y,z and U's together with their σ's if present; only meaningful if IFØRM = 0 or 2.
13 - 15	IØPT	= 0	Read parameters and sigmas from file(s) previously prepared by ØRFFE(FREDFUN)--The file name(s) is (are) TAPE16 and TAPE17.
		= 1	Read parameters and std. errors from cards.
		= 2	Read parameters, but no errors, from cards.

16-18	MERG	= 0	No file merge and no new atom titles.
		= 1	No file merge but read new atom titles from cards.
		= 2	Merge two files (TAPE16 & TAPE17), no new atom names.
		= 3	Merge two files and read new atom names from cards. See Note 3.
19-21	ISCA		A scale factor (input as a power at ten) used to integerise the thermal parameters. Not applied to card output.
22-24	JSCA		Scale factor as above--for the coordinates.

Card(s) 4 Atom parameter cards (if IØPT = 1 or 2)

FØRMAT(A6,21X,3F9.6,/,6F9.6,/,3F12.7,/,6F12.7)

Either two or four cards are read for each atom depending on whether IØPT = 1 or 2. The parameters are: Name,x,y,z,T_{11},T_{22},T_{33}, T_{12},T_{13},T_{23},σ_x,σ_y,σ_z,σT_{11},σT_{22},σT_{33},σT_{12},σT_{13},σT_{23} where T_{ij} is interpreted as either a β_{ij} or a U_{ij} depending on the setting of IFØRM.

Card(s) 5 Alias atom names

FØRMAT(8(A6,4X))

These are read only if MERG = 1 or 3. The atom names supplied here replace those read in with the parameters from either TAPE16 or cards.

Notes

1. The format used for punching the parameters on cards is the same as that used to read them in.

2. If the parameters are to be input from a file prepared by FREDFUN than this must have the filename TAPE16.

3. If the user opts to merge two files then this is done in the following way:

   (i) The atom names read from TAPE16 are retained--those from TAPE17 are rejected.

   (ii) The unweighted mean of the two parameters is used for the final output.

   (iii) The larger of the two standard deviations is chosen for publication.

   If the user wants to change this procedure he can do so by supplying his own version of SUBRØUTINE CØMBIN. Apart from the arbitrary choice of the atom names from TAPE16 over those from TAPE17 these two files are treated the same.

4. The relationship between the β_{ij} terms and the U_{ij} terms is:

$$U_{ij} = \frac{\beta_{ij}}{2\pi^2 a_i^* a_j^*}$$

and so whatever factors (of two) are present in the β's (or U's) then these are also present in the U's (or β's).

G. J. B. Williams May/75

BNL CRYSTALLOGRAPHIC COMPUTER PROGRAM

```
PROGRAM CORDAT(INPUT,OUTPUT,TAPE5=INPUT,TAPE2,TAPE4,TAPE8)
```

THIS PROGRAM READS DATA FROM PROGRAM PROCK OR PROGRAM ABSOR AND APPLIES CORRECTION FACTORS TO GENERATE PROPERLY SCALED VALUES OF FSQ AND SIGFSQ FOR INPUT TO PROGRAMS AVSORT OR FLINUS,ETC. THE EQUATIONS IT USES ARE AS FOLLOWS --

```
      RAWI=SCB*((OBS/SCB)*TAUCOR-(SLO/SLB)*(BAK/SCB))
      FSQ=SCL(N)*(1/LP)*ABSN*RAWI
  RAWSIGSQ=SCB*SCB*((TAUCOR**4)*((OBS/SCB)+(0.5-(1/12))*SLO)
                        + ((TAUCOR*OBS/SCB)**4)*(SIGTAU**2)
            + ((SLO/SLB)**2)*((BAK/SCB)+(0.5-(1/12))*SLB))
      SIGSQI= RAWSIGSQ + (P*RAWI)**2 + (RSIG(N)*RAWI)**2
                       + (Q*RAWI)**2
      SIG(FSQ)=SCL(N)*(1/LP)*ABSN*SQRT(SIGSQI)
```

OBS,BAK,SLO,SLB,SCB ARE PASSED FROM PROCK (SEE PROCK WRITEUP). SCB IS THE NORMALIZATION SCALE FACTOR USED BY PROCK TO PUT ALL REFLECTIONS ON A COMMON SCALE. ABSN IS THE ABSORPTION CORRECTION PASSED FROM ABSOR. TAUCOR IS AN EMPIRICAL CORRECTION FOR DETECTOR DEADTIME (SEE CARD 4 AND SUBROUTINE NETCLC).

THE PROGRAM ALWAYS WRITES A BCD OUTPUT FILE SUITABLE FOR INPUT TO AVSORT. IT CAN ALSO BE TOLD TO WRITE A BINARY FILE FOR INPUT TO FLINUS.

CORDAT WAS WRITTEN BY FLIEG HOLLANDER, JAN. 1975 WITH AID FROM LARRY ANDREWS AND GRAHEME WILLIAMS. IT HAS BEEN MODIFIED (4 FEB 75) TO SCALE SIG(FSQ) CORRECTLY AND TO HANDLE CORRECTLY THE PROCK NORMALIZATION FACTORS (SEE SUBROUTINE NETCLC AND EQUATIONS ABOVE).

********** INPUT CARDS **********

CARD 1 - 8A10 - TITLE
IDENTIFIER FOR THE COMPOUND AND CRYSTAL

CARD 2 - 7F10.6 - A,B,C,ALPH,BET,GAM,ELAM
CELL PARAMETERS AND WAVELENGTH (IN ANGSTROMS)
EITHER REAL OR RECIPROCAL CELL MAY BE INPUT, AND ANGLES MAY BE EITHER IN DEGREES OR EXPRESSED AS COSINES.

CARD 3 - 16I5 - ICN(I),I=1,16
CONTROL INTEGERS -- ONLY THE FIRST SIX ARE USED AT THIS TIME

ICN(1) - COL. 5
= 0, NEUTRON DATA
= 1, X-RAY DATA

```
ICN(2) - COL. 10
      = 0, TAPE2 DATA FROM PROGRAM ABSOR
      = 1, TAPE2 DATA FROM PROGRAM PROCK, WITH *LONG* RECORDS
           CONTAINING THE EXPERIMENTAL REFLECTION NUMBER.
      = 2, TAPE2 DATA FROM PROCK, SHORT RECORD CARD IMAGES.
      = 3, CARD DATA FROM PROCK, SEE CARD SET 8.
ICN(3) - COL. 15
      = 0, NORMAL CASE, NO BINARY FILE WRITTEN.
      = 1, BINARY FILE WRITTEN ON TAPE 8, SUITABLE FOR INPUT
           TO FLINUS
ICN(4) - COL. 16-20
      = 0, MONITOR PRINTOUT OF PROCESSING.  ONLY REJECTED
           REFLECTIONS AND EVERY 100TH ACCEPTED REFLECTION
           WILL BE PRINTED OUT.
      = 1, PRINTOUT OF ALL REFLECTIONS PROCESSED.
      = N, MONITOR PRINTOUT OF PROCESSING.  REJECTED
           REFLECTIONS AND EVERY (N)TH ACCEPTED REFLECTION
           WILL BE PRINTED OUT.
ICN(5) - COL. 21-25
      = 0, NORMAL CASE.
      = N, N REFLECTIONS TO BE REPLACED OR DELETED USING
           CARD SET  7.  UP TO 100 REFLECTIONS ALLOWED.
ICN(6) - COL. 30
      = JSCL - BATCH IDENTIFIER NUMBER REFERENCED BY FLINUS.
           NEEDED IF MORE THAN ONE CRYSTAL USED IN DATA COLL.
           AND IN CERTAIN OTHER CASES.
           IF LEFT BLANK (NORMAL CASE), JSCL = 1.

CARD 4 - 6F10.6 - TTM,P,Q,REJ,TAU,SIGTAU
      TTM = MONOCHROMETER TWO THETA.  NEEDED FOR XRAY DATA,
           IGNORED FOR NEUTRON DATA.
      P = IGNORANCE FACTOR TO INCREASE SIGMAS ABOVE COUNTING
           STATISTIC. NON-POISSON CONTRIBUTION TO SIGMA.
      Q = FRACTIONAL ERROR IN ABSN.  ADDS A TERM TO THE SIGMAS
           TO INCREASE THEM FOR ERROR IN ABORPTION CORRECTION.
       **** SEE EQUATIONS ABOVE FOR FORM OF P AND Q CONTRIBUTION
           TO SIGMA.  IT IS STRONGLY RECOMMENDED THAT P NOT
           BE USED IN IN COMBINATION WITH THE RSIG FACTOR
           AND THAT Q NOT BE USED UNLESS A TRUE MEASURE OF
           THE UNCERTAINTY IN THE ABSORPTION CORRECTION IS
           AVAILABLE.
      REJ = REJECT REFLECTION FROM DATA SET IF FSQ IS NEGATIVE
           AND ABS(FSQ).GE.(REJ*SIGFSQ). IF LEFT BLANK, REJ=5.0
           IF REJ.LT.0.0 THEN ALL NEGATIVE FSQ WILL BE REJECTED
      TAU = EFFECTIVE DEADTIME CONSTANT (MICROSECONDS) AS DET-
           ERMINED BY A LEAST-SQUARES ANALYSIS OF SEVERAL
           REFLECTIONS MEASURED AT DIFFERENT BEAM CURRENTS
           (X-RAY) OR INCIDENT BEAM ATTENUATORS (NEUTRON).
           USED TO SCALE OBS IN THE EQUATIONS ABOVE.
           (ALSO SEE SUBROUTINE NETCLC FOR USE OF TAU,SIGTAU.)
```

SIGTAU = SIGMA OF EFFECTIVE DEADTIME (MICROSECONDS).
ADDS A TERM TO RAWSIGSQ (ABOVE).
NORMALLY BOTH TAU AND SIGTAU ARE ZERO OR BLANK.
***PLEASE NOTE THAT TAU AND SIGTAU ARE STRONGLY
DEPENDENT ON EXPERIMENTAL CONDITIONS, ESPECIALLY
COUNTING TIME PER STEP AND PEAK WIDTH. ***
***DO NOT INPUT TAU AND SIGTAU UNLESS YOU HAVE
DETERMINED THEM EXPERIMENTALLY. ***

CARDS 5 - 8(I5,F5.3) - (NREF(J),SCL(J)),J=1,16 -- TWO CARDS--

REFLECTION NUMBER AND SCALE FACTOR AT THAT NREF. THE SCALE FACTOR WILL BE INTERPOLATED LINEARLY BETWEEN GIVEN NREF(J) BASED ON THE NREF OF THE REFLECTION. NREF(J) MUST BE IN INCREASING NUMERICAL ORDER, BUT THE NREFS OF THE DATA NEED NOT BE SO ORDERED. BOTH CARDS MUST BE PRESENT, BUT FIRST BLANK FIELD TERMINATES APPLICATION OF SCALING. ANY REFLECTION HAVING AN NREF OUTSIDE THE SPECIFIED RANGE WILL BE SCALED BY 1.0. TWO BLANK CARDS GIVE SCALING BY 1.0 TO ALL DATA.

CARDS 6 - 8(I5,F5.3) - (NRSIG(J),RSIG(J),J=1,16) -- TWO CARDS --

REFLECTION NUMBER AND RSIG CONTRIBUTION TO SIGSQI AT THAT REFLECTION NUMBER. RSIG IS THE FRACTIONAL ERROR IN THE (DECAY) SCALE FACTOR DETERMINED FROM THE STANDARDS. SEE EQUATIONS ABOVE FOR THE FORM OF THE CORRECTION. INTERPOLATION AND READING OF THE CARDS IS THE SAME AS FOR CARDS 5, EXCEPT THAT RSIG =0.0 FOR UNSPECIFIED NREF OR TWO BLANK CARDS. A CONSTANT TERM CAN BE INPUT HERE OR WITH P ON CARD 4 -- THE USE OF THESE CARDS TOGETHER WITH P ON CARD 4 IS NOT ADVISED.

SCALING AND RSIG CONTRIBUTIONS CAN BE INPUT FOR SHORT RECORD DATA. THE PROGRAM ASSIGNS NREF IN INPUT ORDER. THIS IS NOT REALLY A GOOD IDEA DUE TO THE WAY THAT PROCK HANDLES THE DATA AND REORDERS IT.

CARDS 7 - 5I5,2F15.3 - IH,IK,IL,NREF,ICODE,RAWI,SIGRAWI

DELETION/REPLACEMENT CARDS -- EXACTLY ICN(5) CARDS -- DO NOT INPUT THIS CARD SET IF ICN(5)=0 .

PROGRAM TESTS TO MAKE SURE THAT IH,IK,IL,AND NREF MATCH, THEN EITHER DELETES (ICODE=-1) THE REFLECTION FROM THE OUTPUT DATA SET OR REPLACES (ICODE=+1) THE NET INTENSITY (RAWI,ABOVE) AND ITS SIGMA (SQRT(RAWSIGSQ),ABOVE) WITH THE VALUES GIVEN ON THE CARD. WHEN SHORT RECORDS ARE INPUT NREF IS NOT TESTED AND THE FIRST OCCURRANCE OF THE H,K,L IS REPLACED OR DELETED. GOOD FOR FIXING UP SOME KINDS OF DATA COLLECTION ERRORS.

CARDS 8 - 3I3,2F10.1,F6.3,3F7.2,2F3.0,2F8.0,I2 -
IH,K,L,OBS,BAK,SCB,OM,PHI,CHI,SLO,SLB,OBSFI,BACKFK,IDENT

CARD INPUT OF DATA FROM PROCK. USE ONLY IF ICN(2)=3 . SEE PROCK WRITEUP FOR DEFINITION OF VARIABLES.

CARD 9 - 999 IN COLUMNS 1-3 -- ENDS READING OF CARD 8 DATA.
999 IS *NOT* WRITTEN ON OUTPUT FILES.

NOTE THAT CARD 1 AND CARD 2 FOLLOWED BY 6 BLANK CARDS INDICATES PROCESSING FOR ABSORPTION-CORRECTED NEUTRON DATA WITH NO DECAY CORRECTION , NO RSIG CONTRIBUTION AND NO DELETION OR REPLACEMENT OF REFLECTIONS. THIS IS THE STANDARD CASE FOR A REASONABLE DATA SET.

***** TAPE FILES ******

TAPE 2 - INPUT FROM PROCK OR ABSOR. (SEE SUBROUTINE IMP)

TAPE 4 - BCD OUTPUT TAPE FOR INPUT TO AVSORT.
FORMAT(I1,I3,2I4,F11.3,F10.3,I3,6F6.3,F8.5)
JEND,IH(3),FSQ,SIGFSQ,JSCL,EXT(7)
JEND=0 FOR REFLECTION DATA, JEND =1 FOR DUMMY RECORD AT END OF DATA.
EXT CONTAINS EXTINCTION INFORMATION FROM ABSOR.

TAPE 8 - BINARY OUTPUT TAPE FOR INPUT TO FLINUS.
4*INT,2*REAL,INT,7*REAL,18*REAL
SAME INFORMATION AS BCD TAPE,
PLUS 18 FIELDS OF PADDING FOR CONSISTENCY WITH FLINUS.
(PADDING IS FILLED WITH 0.0)

13-SEP-75 AUTHOR: H. J. BERNSTEIN
31-DEC-75 REVISED: H. J. BERNSTEIN

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

CDC CYBER 70/74, CDC CYBER 70/76
CDC SCOPE 3.4, CDC SCOPE 2.1

```
PROGRAM DECOL(TAPE99,INPUT,OUTPUT,TAPE1,...,TAPE11)
```

PURPOSE

DECOL IS A PROGRAM TO DECOLATE POOL TAPES WRITTEN AT THE BNL RECF.

LIMITATIONS

11 USER TAPES

LOGICAL UNITS

TAPE99	RECF POOL TAPE
INPUT	CONTROL CARDS FOR THE RUN
OUTPUT	SUMMARY INFORMATION
TAPENN	OUTPUT FOR SAT NN

THE PROGRAM DOES ITS OWN SUBSTITUTION FOR FILES TAPE1 THROUGH TAPE11, AND THUS THESE ARE NOT AVAILABLE FOR USER SUBSTITUTION.

INTRODUCTION

DECOL IS A PROGRAM WRITTEN IN FORTRAN AS A REPLACMENT FOR ORACLE. IT HANDLES TAPES WRITTEN IN THE FORMAT FOR RECF POOL TAPES. SUCH TAPES HAVE DATA FOR MANY USERS MIXED. DECOL ALLOWS THE DATA FOR ONE OR MORE USERS TO BE STRIPPED OFF THE TAPE, ONE FILE FOR EACH USER. EACH INPUT LINE ON THE POOL TAPE IS IDENTIFIED BY A SATELLITE NUMBER RANGING FROM 1 TO 99, CORRESPONDING TO THE SATELLITE COMPUTER USED TO COLLECT THE DATA. THIS NUMBER IS USED TO FORM A FILE NAME TAPE1, TAPE2, ..., TAPE99 ONTO WHICH THE DATA FOR THAT SATELLITE WILL BE WRITTEN.

DECOL IS NOT PARTICULARLY AWARE OF THE EXACT BLOCK STRUCTURE OF THE POOL TAPE, OR OF THE USER TAPES, SINCE DEBLOCKING AND CODE CONVERSION ARE HANDLED BY THE RECORD MANAGER.

PROGRAM CALL

DECOL IS AVAILBLE ON THE CRYSNET PROGRAM TAPES VIA ACCESS AS FOLLOWS

```
ATTACH,ACCESS,ID=CPROGS.
ACCESS(DECOL,ID=CPROGS)
```

THIS THEN ALLOWS THE PROGRAM TO BE EXECUTED. FIRST ONE MUST REQUEST (6000) OR STAGE (7000) THE POOL TAPE AND THE USER TAPES, PROVIDING WHATEVER FILE CARDS ARE NEEDED TO SPECIFY THE BLOCKING. THE POOL TAPE SHOULD HAVE THE FILE NAME TAPE99 AND THE USER TAPES SHOULD HAVE NAMES FORMED FROM "TAPE" AND THEIR SATELLITE NUMBERS. FOR EXAMPLE, ON THE 6000, ONE MIGHT HAVE

```
REQUEST,TAPE99,HD,E,US,S,NT,VSN=NXXXXXX. POOL TAPE
REQUEST,TAPE3,HD,N,S,VSN=NYYYYYY. USER TAPE
FILE(TAPE99,RT=F,BT=K,CM=YES,FL=80,MBL=80,RB=1)
FILE(TAPE3,RT=W,BT=I,MBL=5120)
LDSET(FILES=TAPE99)
LDSET(FILES=TAPE3)
DECOL.
```

WHILE ON THE 7000, ONE WOULD HAVE

```
STAGE(TAPE99,HD,E,US,VSN=NXXXXXX) POOL TAPE
STAGE(TAPE3,POST,HD,N,VSN=NYYYYYY) USER TAPE
FILE(TAPE99,RT=F,BT=K,CM=YES,FL=80,RB=1)
DECOL.
```

OF COURSE, ONE MAY USE PERMANENT FILES INSTEAD OF TAPES.

INPUT DATA

TAPE99 - RECF POOL TAPE DATA

THE DATA ON THIS TAPE CONSISTS OF CODED CARD IMAGES, 80 CHARACTERS PER CARD, WITH ARBITRARY USER DATA IN COLUMNS 1 THROUGH 72, THE SATELLITE NUMBER IN COLUMNS 73 AND 74 (I2), AND A SEQUENCE NUMBER IN COLUMNS 75-80. DECOL CAN SURVIVE BAD SEQUENCE NUMBERS, BUT ALL SEQUENCE NUMBERS AFTER THE FIRST BAD ONE WILL BE TREATED AS ZERO. IN ORDER TO BE STAGED TO THE 7000, THE TAPE MUST BE PROPERLY TERMINATED. IF THIS IS NOT THE CASE, ONE CAN ATTEMPT STAGE BY BLOCK, OR DO THE RUN ON THE 6000.

INPUT - CONTROL CARDS FOR THE RUN

CARD 1 - TITLE - ANY 80 CHARS, PLEASE INCLUDE REEL NO.
CARD 2 - PARAMETERS FOR FIRST USER (I2,2I6,6X,6A10)
SAT NO IN COL 1-2
LOWEST SEQUENCE NO IN COL 3-8
HIGHEST SEQUENCE NO IN COL 9-14
(BLANK IF ALL ARE TO BE TAKEN)
COMMENT IN COL 21-80 (INCLUSE REEL)

FOLLOW WITH ONE SUCH CARD FOR EACH USER

OUTPUT DATA

OUTPUT - RUN SUMMARY INFORMATION

THE OUTPUT FILE CONTAINS A SUMMARY PAGE FOR ALL USERS COLLECTIVELY AND ONE SUMMARY PAGE FOR EACH USER INDIVIDUALLY, GIVING THE NUMBER OF RECORDS ASKED FOR AND WRITTEN ON EACH TAPE. THE SAME INFORMATION IS PLACED IN THE DAYFILE.

TAPENN - DATA FOR SATELLITE NN

EACH USER FILE CONSISTS OF THE LINE IMAGES FOR THAT USER FROM THE RECF POOL TAPE. COLUMNS 1 THROUGH 72 ARE EXACTLY THE SAME, WHILE COLUMNS 73-80 MAY HAVE BEEN SLIGHTLY ALTERED DUE TO WRITING IN I FORMAT. IN PARTICULAR, SEQUENCE NUMBERS MAY HAVE BEEN CHANGED TO ZERO IF A BAD ONE WAS HIT. IF USER SEQUENCE NUMNERS WERE SPECIFIED, THE OUTPUT FOR THAT USER WILL BE RESTRICTED TO CARD IMAGES WITH SEQUENCE NUMBERS WITHIN THE RANGE SPECIFIED.

NOTE

AS OF THIS WRITING, THE RECF DOES NOT WRITE VALID SEQUENCE NUMBERS, AND ALL RUNS WILL INCLUDE AN "ILLEGAL DATA IN FIELD" MESSAGE IN THE OUTPUT WHEN THIS CONDITION IS DETECTED. THIS IS A NON-FATAL ERROR.

Brookhaven Crystallographic Computer Program

NAME: DISCOR TIME: < 20_8 SECS

CORE: $40K_8$

PROGRAM DISCOR (INPUT,OUTPUT,TAPE1,TAPE2).

Purpose: This program is used to obtain bond DIStances CORrected for thermal motion according to the method of W. R. Busing and H. A. Levy, Acta Cryst., 17, 142 (1964). The uncorrected and the "riding motion corrected" distances are output along with the "lower bound" (minimum) and "upper bound" (maximum) bond lengths. It is the user's responsibility to select the best estimator of the bond distance from these.

Input: Four kinds of cards may be input.

A. Title card - FORMAT(8A10)

B. Cell card - cell edge lengths may be in either Å of $Å^{-1}$ and the angles may be either degrees or cosines of angles. FORMAT(6F9.6)

C. Atom parameter cards for each group. Two cards per atom in FLINUS style. Parameters for the "heavy atom" must be first in each group and there must be cards for at least 3 atoms. DISCOR defines an axial system from the coordinates of these three atoms and so they must not be coplanar. If the user wishes to correct a single distance (e.g. $\rightarrow$C-H) for thermal motion then he should supply the C atom, the H atom and any other position (e.g. the cell origin) as the third atom. All three of these atoms should have associated thermal parameter cards which bear sensible coefficients. FORMAT(A6,21X,3F9.6,/,6F9.6)

D. STOP1, STOP2 or STOP3 directives.

After STOP1 follow with another group of cards C from the same structure.

After STOP2 follow with a complete set-up for another structure i.e. cards A,B,C.

After STOP3 is encountered no further computations will occur i.e. this denotes an exit from the program.

DISPOSE IS A CONTROL CARD THAT IS VERY USEFUL IN DIRECTING FILES TO TERMINALS AND SEGMENTING SUCH FILES.

IN GENERAL, THE OUTPUT FILES ASSOCIATED WITH A JOB (BASICALLY OUTPUT AND PUNCH) ARE RETURNED TO THE TERMINAL FROM WHICH THE JOB WAS SUBMITTED OR ARE HANDLED AT THE CENTRAL COMPUTER IF THEY CAME IN FROM THERE. WHEN A JOB REFERENCES OUTPUT OR PUNCH (OR ANY OTHER FILE NAME) A FILE OF THAT NAME IS CREATED IF IT DOES NOT ALREADY EXIST. IT IS A LOCAL FILE WITH AN INDICATOR OF WHERE IT IS TO GO AT JOB COMPLETION.

IF ONE WISHES TO HAVE ONE,S PUNCH FILE GO TO CENTRAL AT JOB COMPLETION ONE WOULD USE

```
6600     DISPOSE(PUNCH,*PU=C)
7600     DISPOSE(PUNCH,ST=MFA,*PU=C)
```

TO DIRECT PRINT FILES TO CENTRAL AT JOB COMPLETION ONE WOULD USE

```
6600     DISPOSE(OUTPUT,*PR=C)
7600     DISPOSE(OUPTUT,ST=MFA,*PR=C)
```

TO DIRECT FILES TO A TERMINAL (AM IN ALL EXAMPLES) AT JOB COMPLETION ONE WOULD USE

```
6600     DISPOSE(PUNCH,*PU=IAM)
6600     DISPOSE(OUTPUT,*PR=IAM)
7600     DISPOSE(PUNCH,ST=MFAIAM,*PU)
7600     DISPOSE(OUTPUT,ST=MFAIAM,*PR)
```

THIS IS ESPECIALLY USEFUL FOR JOBS SUBMITTED AT SOME OTHER TERMINAL OR CENTRAL.

IT IS MOST IMPORTANT TO REMEMBER THAT DISPOSE CARDS MUST BE PLACED IN THE CONTROL CARD DECK IN SUCH A POSTION THAT THEY WILL BE EXECUTED UNDER THE PROPER CIRCUMSTANCES. IN ADDITION, DISPOSE CAN BE USED FOR FILES OTHER THAN PUNCH AND OUTPUT. THE PU MEANS PUNCH, PR MEANS PRINT. ALL FILES WILL BE GIVEN A NAME IDENTICAL TO THE JOB NAME.

BY REMOVING THE * IN ANY OF THE FORMS ABOVE ONE TELLS THE SYSTEM TO PERFORM THE ACTION NOW INSTEAD OF WAITING FOR JOB COMPLETION. THE FILE, AS IT IS NOW WHEN THE DISPOSE IS ENCOUNTERED, IS GIVEN THE JOB NAME AND DISPOSED. A NEW PUNCH OR OUTPUT FILE WILL BE STARTED AT NEXT USE IN THIS JOB. THIS IS AN EFFECTIVE METHOD OF SPLITTING A LARGE OUTPUT FILE, SENDING PARTS OF IT TO A TERMINAL OR CENTRAL. BY ESTABLISHING A COMPLEX SEQUENCE OF CONTROL CARDS ONE CAN BE QUITE FLEXIBLE.

EXAMPLE

```
D555X.   6600 JOB
ACCOUNT...
FTN(A)   A FORCES ABORT ON COMPILATION ERRORS
DISPOSE(OUTPUT,OUTPUT,PR=C)  SEND COMPILATION LISTING TO
          CENTRAL FOR LATER DELIVERY IF NO COMPILATION ERRORS
LGO.
DISPOSE(PUNCH,PU=C)  SEND PUNCH TO CENTRAL IF EXECUTION OK
EXIT.
DISPOSE(PUNCH)  ELIMINATE PUNCH ALTOGETHER IF ANY ERRORS
```

IN THIS EXAMPLE, IF THERE ARE NO ERRORS THE COMPILATION LISTING AND PUNCH GO TO CENTRAL FOR DELIVERY AND THE EXECUTION OUTPUT PLUS DAYFILE

GOES TO THE ORIGINATING TERMINAL.

EXAMPLE

```
D555X,CP70,TP0.  7600 JOB
ACCOUNT...
FTN.
LGO.
BKSP(*,*) FORCE ERROR TO SEND CONTROL AFTER EXIT. CARD
EXIT.
DISPOSE(OUTPUT,ST=MFA,PR=C)
```

HERE THE ENTIRE OUTPUT EXCEPT THE DAYFILE IS SENT TO CENTRAL.

EXAMPLE

```
D555X,CP70,TP0.  7600 JOB
ACCOUNT...
FTN.
LGO.
BKSP(*,*)
EXIT.
DISPOSE(OUTPUT,ST=MFAIAM,PR)
DISPOSE(OUTPUT,ST=MFAIAM,*PR)
```

ONLY THE DISPOSE CARDS DIFFER FROM THE PREVIOUS EXAMPLE. THE FIRST DISPOSE SENDS THE ENTIRE OUTPUT EXCEPT FOR THE DAYFILE TO TERMINAL AM. THE SECOND SAYS TO SEND THE OUTPUT FILE AT JOB COMPLETION TO AM BUT IN THIS CASE THE OUTPUT FILE CAN ONLY CONTAIN THE DAYFILE AT JOB COMPLETION. THUS THE DAYFILE IS SEPARATED FROM THE JOB AND CAN BE PRINTED SEPARATELY. FOR LARGE OUTPUT FILES ONE CAN THUS EXAMINE THE DAYFILE FIRST AND THEN DECIDE WHEN AND WHERE TO PRINT THE OTHER OUTPUT. THIS SHOULD BE USED WITH CARE SINCE BOTH FILES WILL HAVE THE SAME NAME AND ARE DIFFICULT TO MANIPULATE AT THE TERMINAL BECAUSE MOST COMMANDS (PRIOR,DIVERT,EVICT,ETC) AFFECT ALL FILES OF THE SAME NAME IN THE TABLE. IF THE LARGE FILE GETS TO THE PRINTER FIRST ONE CAN THEN DO RTN,NNN WHERE NNN IS A PRIORITY CHOSEN TO BE LESS THAN THAT OF THE DAYFILE.

FURTHER DETAILS CAN BE FOUND IN THE SCOPE 2.1 AND 3.4 REFERENCE MANUALS OR BY ASKING FRANCES C. BERNSTEIN

EDIT

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

CDC CYBER 70/74, CDC CYBER 70/76
CDC SCOPE 3.4, CDC SCOPE 2.1

PROGRAM EDIT(ZZZZZA,ZZZZZB,ZZZZZC,ZZZZZD,INPUT=ZZZZZA,TAPE1=ZZZZZB,
TAPE2=ZZZZZC,OUTPUT=ZZZZZD,TAPE3=ZZZZZA,TAPE4=ZZZZZD)

PURPOSE ...

THIS PROGRAM IS A CONTEXT EDITOR WHICH ALLOWS THE USER TO PERFORM BOTH LINE BY LINE AND CONTEXT EDITING OF A TEXT (BCD) FILE SUCH AS A SOURCE PROGRAM, OUTPUT LISTING OR DATA. THIS PROGRAM WAS ORIGINALLY WRITTEN TO EMULATE THE 3200 FOCUS EDITOR ON A 6600 COMPUTER AS A BACKUP EDITOR. HOWEVER, THE DEVELOPMENT OF THE PROGRAM REVEALED SO MANY POTENTIAL IMPROVEMENTS AND APPLICATIONS ARISING FROM THESE IMPROVEMENTS THAT THE PROGRAM HAS STAND-ALONE VALUE. IT HAS SINCE BEEN BACK CONVERTED TO RUN INTERACTIVELY UNDER INTERCOM.

THE LANGUAGE USED IS A SUPERSET OF THE FOCUS EDIT COMMANDS. MOST OF THE FOCUS EDIT COMMANDS OPERATE ESSENTIALLY THE SAME EXCEPT FOR THE N COMMAND, WHICH HAS BEEN REDEFINED, AND THE GLOBAL COMMAND WHICH HAS BEEN EXPANDED TO INCLUDE ANOTHER TEST CONDITION AND A LOOP NESTING CAPABILITY. FURTHERMORE, ALMOST ALL RESTRICTIONS HAVE BEEN DROPPED AND SIX NEW COMMANDS PLUS A COMMENTS FEATURE HAVE BEEN ADDED. THESE IMPROVEMENTS HAVE GREATLY EXPANDED THE POWER AND VERSATILITY OF THE EDITOR LANGUAGE.

THOSE USED TO THE PRIOR BNL SCOPE VERSION SHOULD NOTE THAT THE J COMMAND HAS BEEN CHANGED BACK TO AGREE WITH THE FOCUS MEANING AND THAT IN ORDER TO ALLOW USE INTERACTIVELY UNDER INTERCOM, THE FILE HANDLING IS DIFFERENT. IN PARTICULAR, THE LINE LENGTH MUST BE GIVEN IN THE INPUT DATA (2-3 DIGITS ON THE FIRST LINE TERMINATED BY A COMMA, SIMPLY AS THE FIRST CARD IN BATCH AND AS A RESPONSE TO "NC =" UNDER INTERCOM) AND NOT ON THE CONTROL CARD, WHILE FOR BATCH USE, ALL FILES INCLUDING INPUT AND OUTPUT MUST BE GIVEN EXPLICITLY ON THE CONTROL CARD.

USAGE ...

THE PROGRAM IS AVAILABLE AS A CATALOG FILE WITH PFN EDIT, AND ID=CPROGS. THE PROGRAM REQUIRES NO MORE THAN 30000 CM WORDS TO EXECUTE ON THE CDC CYBER 70/74, AND LESS THAN THAT ON THE CYBER 70/76. THE TIME REQUIRED TO EDIT A FILE CAN VARY WIDELY ACCORDING TO THE SIZE OF THE FILE AND THE MEDIUM (TAPE OR DISK), THE LINE LENGTH SPECIFIED (MAX=135), THE NUMBER OF PASSES BETWEEN THE TEST AND WORK FILES, AND THE COMMAND SEQUENCES.

METHOD ...

THE PROGRAM IS ESSENTIALLY A COMPILER/INTERPRETER FOR A SIMPLE TEXT EDITING CONTROL LANGUAGE WHICH OPERATES ON A LINE-AT-A-TIME BASIS. EACH INPUT LINE CONTAINS A SEQUENCE OF EDIT COMMANDS WHICH DIRECT THE EDITING OF A TEXT FILE. EACH LINE IS SEPARATELY CHECKED FOR SYNTAX, COMPILED, AND THEN EXECUTED IN INTERPRETER MODE.

THE TEXT FILE IS EDITED TO A WORK FILE (WHICH MAY BE THE END PRODUCT), AND UPON COMMAND (P), MAY BE COPIED BACK TO THE SOURCE FILE FOR FURTHER EDITING. THIS PROCESS MAY BE REPEATED UNTIL THE DESIRED RESULT IS ACCOMPLISHED. BOTH FILES ARE REWOUND AT COMPLETION AND EITHER MAY BE USED AS THE END PRODUCT DEPENDING ON THEIR CONTENT.

LANGUAGE DESCRIPTION ...

EACH EDIT COMMAND LINE MAY CONTAIN A SERIES OF COMPLETE EDIT COMMANDS OPTIONALLY PRECEEDED OR SEPARATED BY BLANKS AND/OR COMMENTS. EDIT COMMANDS ARE EXECUTED IN A LEFT TO RIGHT SEQUENCE EXCEPT WHEN MODIFIED BY GLOBAL COMMAND LOOPS. COMMENTS BEGIN AND END WITH A * AS A DELIMITER. IF NO COMMANDS FOLLOW COMMENTS, THE FINAL DELIMITER IS OPTIONAL. COMMENTS AND BLANKS OUTSIDE OF COMMANDS ARE IGNORED.

AN EDIT COMMAND CONSISTS OF A SINGLE LETTER CODE FOLLOWED BY SOME SYNTAX STRUCTURE. SOME COMMANDS REQUIRE A SINGLE MODIFIER LETTER TO FURTHER DEFINE THE COMMAND WHILE OTHERS ALLOW AN OPTIONAL UNSIGNED DECIMAL NUMBER TO PROVIDE A REPETITION COUNT. SEVERAL COMMANDS REQUIRE ONE OR TWO TEXT STRINGS TO DO TEXT PATTERN MATCHING AND REPLACEMENT OR INSERTION. A TEXT STRING IS DEFINED AS THE SERIES OF CHARACTERS BETWEEN TWO OCCURANCES OF A DELIMITER CHARACTER. A DELIMITER CHARACTER IS DEFINED AS THE CHARACTER WHICH IMMEDIATELY FOLLOWS THE COMMAND CODE AND MAY BE ANY CHARACTER, INCLUDING A BLANK. WHEN TWO TEXT STRINGS ARE REQUIRED, THE FIRST STRING INCLUDES ALL CHARACTERS BETWEEN THE FIRST AND SECOND OCCURENCES OF THE DELIMITER AND THE SECOND STRING INCLUDES THOSE BETWEEN THE SECOND AND THIRD OCCURENCES. A NULL OR EMPTY STRING IS DEFINED BY ADJACENT DELIMITERS.

A LOOPING MECHANISM IS PROVIDED IN THE GLOBAL (G) COMMAND SUPERSTRUCTURE WHICH ALLOWS THE USER TO DEFINE CONDITIONAL COMMAND LOOPS. THE CAPABILITY FOR NESTING LOOPS TO 8 LEVELS IS PROVIDED. THE GLOBAL COMMAND STRUCTURE TAKES TWO FORMS ...

```
G<COND><SEQ>
G<COND>(<SEQ>)<EXIT>
```

IN THE FIRST FORM (ORIGINAL SYNTAX), THE LOOP SEQUENCE <SEQ> CONTAINS ALL SUBSEQUENT COMMANDS ON THE SAME LINE AND DOES NOT ALLOW NESTING OR AN EXIT SEQUENCE OF COMMANDS. IN THE SECOND FORM <SEQ> IS DELIMITED BY BALANCED PARENTHESIS AND MAY BE FOLLOWED BY AN EXIT SEQUENCE (BOTH MAY INCLUDE NESTED LOOPS). THE PARENTHESES ENCLOSING THE LOOP SEQUENCE ARE A SPECIAL SYNTAX CASE. THE LEFT PAREN IS REQUIRED FOR ALL INNER LOOPS AND IS PART OF THE INITIATION SYNTAX SUCH THAT NO BLANKS MAY APPEAR FROM THE G THROUGH THE TEST CONDITION TO THE LEFT PAREN. THE RIGHT PAREN APPEARS AFTER A SEQUENCE OF COMMANDS, WHICH MAY CONTAIN INNER LOOPS, AT

THE SYNTAX LEVEL OF A COMMAND CODE. THE ASSOCIATION OF LEFT AND RIGHT PARENTHESES OF A LOOP FOLLOWS THE RULES OF ALGEBRA FOR PARENTHETICAL EXPRESSIONS.

THE GLOBAL <COND> DEFINES THE CONDITION FOR TERMINATING THE LOOP SEQUENCE AND TAKES ONE OF FOUR FORMS ...

L<STR> ... TO LINE BEGINNING WITH <STR>
T<STR> ... TO LINE CONTAINING <STR>
E ..... TO END OF FILE OR END OF LINE
<NUM> .... COUNT TO <NUM> TIMES THROUGH LOOP

THE THIRD FORM EXITS ON ENCOUNTERING THE END OF FILE ON TAPE1 OR, IF NO LINE ADVANCING COMMANDS ARE IN <SEQ>, ON THE END OF THE LINE. THE LAST FORM COUNTS THE NUMBER OF TIMES THROUGH THE LOOP AND EXITS AFTER <NUM> TIMES.

THE EXECUTION OF A GLOBAL COMMAND SEQUENCE OBEYS THE FOLLOWING ...

1. FIRST, A TEST OF THE <COND> IS MADE AND IF MET, THE LOOP IS BYPASSED AND THE CORRESPONDING <EXIT> SEQUENCE IS EXECUTED. OTHERWISE THE LOOP SEQUENCE IS EXECUTED.

2. WHILE IN THE LOOP, EACH NEW DATA LINE IS TESTED FOR THE L<STR> AND T<STR> CONDITIONS FOR EACH INITIATED LOOP BEGINNING WITH THE OUTERMOST FIRST. THIS ALLOWS HONORING EXIT CONDITIONS OF OUTER LOOPS WHEN INNER LOOP CONDITIONS ARE A SUBSET OF AN OUTER CONDITION.

3. FOR AN END OF FILE CONDITION, THE EXIT SEQUENCE OF THE FIRST OUTER GE TYPE LOOP, WORKING OUTWARD, IS TAKEN.

4. UPON REACHING THE END OF A LOOP SEQUENCE, FOR A G<NUM> LOOP THE COUNT IS DECREMENTED, AND EXECUTION IS RESUMED AS IN RULE 1.

5. IF AT ANY TIME, A COMMAND CANNOT BE EXCUTED, THE EXECUTION OF THAT EDIT LINE IS TERMINATED AND THE NEXT EDIT COMMAND LINE IS EXECUTED. THIS MAY BE USED TO ADVANTAGE IN SOME CASES, BUT CARE MUST BE TAKEN THAT THE COMMANDS ON A LINE DO NOT DEPEND ON THE SUCCESSFUL EXECUTION OF COMMANDS ON A PREVIOUS LINE.

6. WHEN A SYNTAX OR LOGICAL ERROR IS ENCOUNTERED IN THE COMPILATION OF A COMMAND LINE AN ERROR MESSAGE IS PRODUCED AND FURTHER PROCESSING IS TERMINATED WITH AN ABORT FROM THE PROGRAM.

THE RULES OF SYNTAX AND USAGE OF THE COMMANDS IS GIVEN IN THE FOLLOWING SYNOPSIS WHICH IS DESIGNED TO BE A CONDENSED USER-S MANUAL.

EDIT - CONTEXT EDITOR

```
PROGRAM CALL .. ATTACH(EDIT,EDIT,ID=CPROGS)
                EDIT.  -- FOR USE UNDER ITERCOM
                EDIT(INPUT,TAPE1,TAPE2,OUTPUT) --  BATCH MODE
  INPUT .. EDIT COMMANDS (130 CHAR/LINE)
  TAPE1 .. TEXT FILE TO BE EDITED (MAY BE REWRITTEN)
  TAPE2 .. WORK FILE OR END RESULT
  OUTPUT .. RUNNING COMMENTARY AND DIAGNOSTICS

UNDER INTERCOM ASKS FOR FILE TO EDIT
FIRST INPUT COMMAND MUST BE CHAR/LINE (MAX=135=DEFAULT) IN ANY CASE.


  -COMMAND-        -NOTE- -SEMANTICS-
  A<STR1><STR2>    3,4,6  AFTER <STR1> INSERT <STR2>
  B<STR1><STR2>    3,4,6  BEFORE <STR1> INSERT <STR2>
  C[<NUM>]         7      COPY [NUM> LINES TO TAPE2
  D[<NUM>]         7      DELETE [NUM> LINES
  E                4      SKIP TO EOF ON TAPE1
  F                2,4    FIND END OF CURRENT LINE
  G<COND><SEQ>     9      GLOBAL EDIT LOOP SEQUENCE UNTIL CONDITION MET
  G<COND>(<LOOP>)<EXIT>
                   2      GLOBAL EDIT LOOP WITH NESTING AND EXIT SEQUENCE
  H                2      HOLD TEXT COPIED AND SKIP TO NEXT LINE
  I<STR>           4,8    INSERT LINE <STR> BEFORE START OF LINE
  J                       RESTART CURRENT EDIT PASS
  K[<NUM>]         2,7    COPY <NUM> CHARACTERS TO TAPE2 LINE
  L<STR>           4,6,8  LOCATE LINE BEGINNING WITH <STR>
  M                8,9    MULTI-LINE INSERT FROM INPUT UNTIL BLANK LINE
  N                1      NEW SCAN OF TAPE1 LINE (TAPE2 LINE SAVED)
  O                       PRINT CURRENT LINE (USED IN UNVERIFY MODE)
  P                4      SKIP TO EOF TAPE1, COPY TAPE2 BACK TO TAPE1.
  Q                9      QUIT EDITING, CLOSE AND REWIND FILES
  R<STR1><STR2>    3,4,6  REPLACE <STR1> WITH <STR2>
  S<MODE>                 SET MODE .. C = COPY (DEFAULT), D = DELETE MODE
  T<STR>           4,6    SCAN TO LINE CONTAINING TEXT <STR>
  U                       UNVERIFY MODE
  V                5      VERIFY MODE
  W                2      WRITE OUTPUT LINE BUFFER ONLY (NO ADVANCE)
  X[<NUM>]         2,7    IGNORE <NUM> CHARACTERS OF INPUT LINE
  Z                2      ZERO (CLEAR) OUTPUT LINE BUFFER ONLY
  *<COMMENTS>[*]
                          IGNORED, 2ND * REQUIRED FOR FOLLOWING COMMANDS


LEGEND
  [X] ..... DENOTES X IS OPTIONAL
  <NUM> ... AN UNSIGNED DECIMAL NUMBER
  <STR> ... A CHARACTER STRING BRACKETED BY A DELIMITER CHARACTER
  <COND> ... EXIT TEST ... E (TO EOF), L<STR>, T<STR>, OR <NUM> TIMES
  THROUGH
  <SEQ> ... A COMMAND SEQUENCE EXCLUDING G, M, AND Q
  <LOOP> .. A LOOP COMMAND SEQ INCLUDING INNER LOOPS, EXCLUDING M, Q
  <EXIT> ... EXIT COMMAND SEQUENCE INCLUDING ANY OUTER LOOP SEQUENCE
```

NOTES

1 - COMMAND REDEFINED FROM FOCUS EDIT
2 - COMMAND ADDITIONAL TO FOCUS EDIT
3 - ONLY ONE <STR> MAY BE EMPTY
4 - LINES/CHARACTERS SKIPPED ARE NOT COPIED IF IN DELETE MODE
5 - INITIAL DEFAULT MODE
6 - A STRING MATCH MAY INCLUDE BLANKS EXTENDING PAST END OF LINE
7 - <NUM> = 1 IF NOT SPECIFIED
8 - IF NOT AT START OF LINE, POINTER IS ADVANCED TO NEXT LINE
9 - NO MORE COMMANDS MAY FOLLOW

NAME: EFACTH

AUTHOR: F. Bernstein

CORE: $30K_8$ or $40K_8$ (if replacement subroutines used)

DATE: January 1974

PROGRAM EFACTH(INPUT,ØUTPUT,PUNCH,DATA,SHØRT,ERRMSG,TAPE5=INPUT,TAPE6=ØUTPUT,
TAPE7=PUNCH,TAPE12=DATA,TAPE14=SHØRT,TAPE15=ERRMSG)

I. PURPOSE:

To calculate normalized structure factors (E).

II. TAPES:

A. DATA-Binary Purpose-input Format-ISENT,FH,FK,FL

III. LIMITATIONS:

A. Number of atom types. Dimension-12

IV. REPLACEABLE SUBROUTINES:

	ARGUMENT
A. IMP - reads input data	FH,FK,FL,FOBS,ISENT
B. MOMENT - puts in correct epsilon if space group is not $P2_1/a$, $P2_1/c$	FH,FK,FL,DEVIDE

V. DECK SET UP

A. JOB CARD
1. TIME LIMIT - ∿100 secs
2. FIELD LENGTH - $40K_8$
3. NUMBER OF TAPES - 1
4. ECS - none

B. CONTROL CARDS

```
ATTACH(EFACTH,EFACTH,ID=CPRØGS)
FTN(SYSEDIT)                      NOTE: If supplying subroutine.
REQUEST(DATA,,,,)                 NOTE: If input on tape.
LØAD(LGØ)                         NOTE: If using subroutine.
EFACTH.
```

C. DATA CARDS:

CARD	FORMAT
1. Serial#,title card	I5,9A6
2. Cell constants	6F10.6,2I5
3. Scale,temp.,etc.	2F10.5,I2,I3,2I5,4F10.5
4. Scattering factor cards	7(F4.2,F6.3) or LINUS format
5. Number of atoms	12F5.0
6. (Data)	I4,F3.0,2F4.0,F9.3 if data on cards

D. REMOTE FILES:

ERRMSG
SHØRT
ØUTPUT
PUNCH

```
      PROGRAM EFACTH(INPUT,OUTPUT,PUNCH,DATA,SHORT,ERRMSG,TAPE5=INPUT,
     1TAPE6=OUTPUT,TAPE7=PUNCH,TAPE12=DATA,TAPE14=SHORT,TAPE15=ERRMSG)
C
C     FRANCES C. BERNSTEIN  9/73  BNL
C     GENERATE VERY SHORT FILE ERRMSG AND MEDIUM FILE SHORT FOR
C     CONVENIENCE FOR REMOTE USERS
C
C     DATA IS THE INPUT TAPE
C     IMP ROUTINE SUPPLIED READS CLINUS OR FLINUS DATA TAPE, I.E.
C     ECSORTH OUTPUT TAPE
C5A EFACT-GENERATES E-FACTORS
C  6600/7094/7040//FORTRAN4///BEDNOWITZ,A.L.//
C  BROOKHAVEN NATIONAL LABORATORY.  UPTON, N.Y. 11973
C    GIVEN AN ABSOLUTE SCALE FACTOR(K=FOBS/FCAL) AND A MEAN ISOTROPIC
C  TEMPERATURE FACTOR THIS PROGRAM WILL GENERATE THE STANDARD NORMALIZED
C  STRUCTURE FACTOR OR E-FACTOR ON BCD TAPE OR PUNCHED OUTPUT.
C                         INPUT INSTRUCTIONS
C*************************************************************************
C     OPTIONAL INPUT REQUEST FILE DATA
C*****************************************
C*****************************************
C      EFACT    GENERATES THE E-FACTORS FROM OBSERVED DATA.
C      EWALD   WILL COMPUTE RECIPROCAL CONSTANTS FROM THE DIRECT VALUES.
C      MULT    TWO SUBROUTINES, MULT2 AND MULT3 FOR MULTIPLICITY.
C      MOMENT  FOR THE DETERMINATION OF THE EPSILON FACTOR. VARIABLE SUB
C      IMP     VARIABLE SUBROUTINE FOR TAPE OR CARD INPUT.
C*************************************************************************
C                         INPUT DATA
C*************************************************************************
CITEM  1       1FORMAT(I5,9A6)
C1-5   NSERI   SERIES NUMBER FOR KEEPING TRACK OF COMPUTATIONS.
C6-70  COMPD   (COMPD(I) I=1,9)   COMPOUND NAME
C*************************************************************************
CITEM  2       2FORMAT(6F10.6,2I5)
C1-10  A       EITHER A AXIS REPEAT OR 1/D(100)
C11-20 B       EITHER B AXIS REPEAT OR 1/D(010)
C21-30 C       EITHER C AXIS REPEAT OR 1/D(001)
C31-40 COSA    COSINE OF ALPHA OR ANGLE BETWEEN (001) AND (010).
C41-50 COSB    COSINE OF BETA  OR ANGLE BETWEEN (001) AND (100).
C51-60 COSC    COSINE OF GAMMA OR ANGLE BETWEEN (100) AND (010).
C61-65 NREC    .EQ.0 FOR DIRECT LATTICE CONSTANTS.
C              .GT.0  FOR RECIPROCAL INPUT.
C66-70 ISFOBS  .GT.0 IF INPUT COEFFICIENTS ARE F**2. .LE.0 IF THEY ARE F
C71-80 SOLMAX  MAXIMUM SIN(THETA)/LAMBDA TO BE USED IN THIS PROGRAM.
C              IF ZERO THEN SOLMAX IS SET TO 2.0
C*************************************************************************
CITEM 3        3FORMAT(2F10.5,I2,I3,2I5,4F10.5)
C1-10  SCALE   ABSOLUTE SCALE FACTOR FROM WILSON STATISTICS, K=FOBS/FCAL
C11-20 BTEMP   TEMPERATURE FACTOR FROM WILSON STATISTICS.
C21-22 IWFORM  IF .GT. 0 USE CLINUS FORMAT FOR FORM FACTORS,
C              4 CARDS PER TABLE
C              IF .EQ. 0 USE FORM FACTOR TABLES IN FORMAT SPECIFED BELOW
C23-25 NTBL    NO. OF F TABLES INPUT, I.E. THE NUMBER OF DIFFERENT ATOMS
C26-30 NPUNCH  IF .GT. 0 PUNCH H,K,L,EFACTORS
C31-35 NFORM   IF .LE. 0 PUNCH FORMAT IS (3I5,F5.3)
C              IF .GT. 0 READ ITEM 6 FORMAT FOR PUNCH - UP TO 80 CHARS
C36-40 INTAPE  IF .GT. 0 REFLECTION DATA IS READ BY IMP SUBROUTINE.
```

```
C                   IF .LE. 0 READ ITEM 7 DATA CARDS IN ECSORTH FORMAT
C41-50 WLOLIM       LOWER LIMIT ON THE E-FACTORS TO BE LISTED ON SYSOUT.
C51-60 WUPLIM       UPPER LIMIT ON THE E-FACTORS TO BE LISTED ON SYSOUT.
C61-70 PLOLIM       LOWER LIMIT ON THE E-FACTORS TO BE PUNCHED OR TAPED.
C71-80 PUPLIM       UPPER LIMIT ON THE E-FACTORS TO BE PUNCHED OR TAPED.
C                   IF ALL E-FACTORS ARE DESIRED ON THE LIST AND/OR PUNCH OUT
C                   LEAVE THE LAST FOUR VARIABLES BLANK.
C*******************************************************************
CITEN 4             4FORMAT(7(F4.2,F6.3))
C                   THREE CARDS FOR EACH TYPE OF ATOM
C                       (SLAM(I,J),FTBL(I,J),J=1,21)
C                   21 VALUES OF SIN(THETA) VS ATOMIC SCATTERING FACTOR
C*******************************************************************
CITEM5              5FORMAT(12F5.0)
C                   (FOATOM(I),I=1,NTBL)
C                   THE NUMBER OF EACH TYPE OF ATOM IN ORDER OF ITS F TABLE
C                   MAXIMUM NUMBER OF DIFFERENT ATOMS IS 12.
C*******************************************************************
C**** REFLECTION DATA STANDARD CARD INPUT FORMAT WHEN INTAPE .LE.0
CITEM 7             4FORMAT(I4,F3.0,2F4.0,F9.3)
C                   REFLECTION DATA INPUT
C1      ISENT       = 0 NORMALLY
C                   = 1 TO TERMINATE
C2-4    FJ          H VALUE
C5-8    FK          K VALUE
C9-12   FL          L VALUE
C13-21  FOBS        FOBS OR IOBS VALUE
C**** WHEN INTAPE .GT. 0 THE TERMINATION INDICATOR ISENT=1 MUST BE SET
C       BY THE IMP SUBROUTINE. INPUT MAY BE IN ANY FORM.
C*******NOTE******
C       IF THE SPACE GROUP IS OTHER THAN TRICLINIC, MONOCLINIC OR
C       ORTHORHOMBIC THE SUBROUTINE MULT WILL HAVE TO BE MODIFIED.
C       NOTE WELL THAT MULTIPLICITY FACTORS ARE DETERMINED BY LOOKING AT
C       COSINES OF CELL ANGLES.  IF ALL ARE ZERO, CELL IS ASSUMED TO BE
C       ORTHORHOMBIC.  IF COS ALPHA AND COS GAMMA ARE ZERO BUT COS BETA
C       IS NOT, CELL IS ASSUMED TO BE MONOCLINIC.  IF COS ALPHA OR COS
C       GAMMA IS NOT ZERO, CELL IS ASSUMED TO BE TRICLINIC.
C************************
C************************
C
C       IF NPUNCH.GT.0 THEN THE E-FACTORS ARE PUNCHED OUT.
C       TO OBTAIN BCD TAPE OUTPUT, REPLACE FILE PUNCH ON THE PROGRAM
C       EXECUTION CARD BY A FILENAME WHICH CAN BE ASSIGNED TO A
C       PHYSICAL TAPE.
```

```
      SUBROUTINE MOMENT(FH,FK,FL,DEVIDE)
C      FOR THE SPACE GROUPS P21/A,P21/C, OR P21/N.
      IF(FH.EQ.0.,AND.FL.EQ.0.) DEVIDE = 2*DEVIDE
      IF(FK.EQ.0.)DEVIDE = 2*DEVIDE
   10 RETURN
      END
```

```
      SUBROUTINE IMP(FJ,FK,FL,FOBS,ISENT)
      READ(12) ISENT,FJ,FK,FL,FOBS
      RETURN
      END
```

Brookhaven Crystallographic Computer Program Writeup

NAME: EXAMØR FILES: 4 TIME: 4 sec/1000 refl.

Core: 25K

Purpose: Process tapes written by ØRACLE to remove garbage reflections that bomb PRØCK

PRØGRAM EXAMØR(INPUT=110,ØUTPUT,TAPE1=750,ØRACLE=750,
TAPE2=ØRACLE,TAPE5=INPUT,TAPE6=ØUTPUT)

Input:

Card 1 (2I5)

col.	1-5	NF number of files to process
	6-10	NR number of records to process (used only if NF=0)

Use:

NF and NR both equal to zero causes the program to read to double EOF (or EOT). Program always stops at double EOF. A tape with local file name ØRACLE is read and TAPE1 is written for input to PRØCK. TAPE1 will consist of a single file regardless of the number of files on the ØRACLE tape. For reflections with bad data nothing is written on TAPE1 and a brief summary is written on OUTPUT. In the summary are:

H,K,L	indices found on tape
2THETA	the value of 2theta found on tape
NO.PTS.	the recorded number of points in the scan
INDEX	the number of the first element which contained illegal data
BAD DATUM	the octal value found in the field specified by INDEX

Possible values for INDEX and their meaning are:

INDEX	CONTENTS(INDEX)
11	H
12	K
13	L
14	STEP SIZE (in .01 degrees)

15	Monitor counts
16	No. points on each side used in the background determined in AXDA/ANDA
17	Scan range measured in .01 of a degree
18	Attenuator scale factor
19	No. of points in scan (NP)
20	Total counts accummulated in scan
21	Total counts in background obtained by approximate integration by AXDA/ANDA
22	Phi (measured in .01 degree)
23	Omega (measured in .01 degree)
24	Two theta (measured in .01 degree)
25	Chi (measured in .01 degree)
29 to 28+NP	Data for NP steps

Brookhaven Crystallographic Computer Program Writeup

NAME: FACES FILES: 2 TIME < 10 sec

CORE FL: 37K

Purpose: An aid in defining crystal geometry by calculating equations of crystal surface planes and their distances from the origin. (It may also be used for finding unweighted best planes through atoms.)

PROGRAM FACES (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)

Input:

Card 1. Scaling (lattice) parameters (6F10.4)

column	content
1-10	x scale constant
11-20	y " " (usually same as x)
21-30	z " " (" " " ")
31-40	the angle, or its cosine, between y and z axes
41-50	" " " " " " x " z "
51-60	" " " " " " x " y "

Note that these parameters may be used to apply a scale factor to the lattice used in defining the coordinates.

Card 2. Number of vertices for plane (I5) (May be zero - but card must be present)

column	content
1-5	number of points to define the plane, 30 maximum (one per card)

Card 3. Coordinates of vertices (3F10.4) (Omit if No. of vertices = 0)
One card for each vertex, up to the number of cards specified on card 2.

column	content
1-10	x coordinate
11-20	y coordinate
21-30	z coordinate

Cards 2 and 3 may be repeated in groups, for up to a total of 30 planes.

Card 4. Real-space cell FORMAT(6F9.6) } Used to obtain a picture of the
Card 5. h,k,ℓ,dist FORMAT(4F10.4) } crystal as described by these cards.

Note: Cards 4 and 5 are used in the PDP 11 version only.

4

Output:

The scaled distance from the origin to the best plane and the direction cosines of the normal to the plane are listed. Each vertex is listed with its distance from the best plane. The angle(s) between the normal to the current plane and the normals of all previous planes are also listed.

Method:

The inertia tensor (T) of the input points about their center of mass is calculated. The best plane is sought by finding the eigenvector of the largest eigenvalue of the inertia tensor.[1] The power method[2] is used to determine the eigenvector. If the dot product of the determined eigenvector and the vector to the center of mass is negative, the eigenvector is inverted through the origin. The distance of the plane from the origin is the dot product of that eigenvector and the vector to the center of mass. The distance of each point from the plane is

$$\text{dist} = (x, e_o) - ||cm||$$

where $||cm||$ is the modulus of the vector to the center of mass, X is the vector to the desired point and e_o is the eigenvector normal to the plane (all vectors are defined as originating at the origin).

$$T = \begin{pmatrix} \sum(y_i^2+z_i^2) & -\sum x_i y_i & -\sum x_i z_i \\ -\sum x_i y_i & \sum x_i^2+z_i^2 & -\sum y_i z_i \\ -\sum x_i z_i & -\sum y_i z_i & \sum(x_i^2+y_i^2) \end{pmatrix}$$

where x_i, y_i, and z_i are referred to the center of mass.

If the inertia tensor is written as:

$$T = \begin{pmatrix} A & -H & -G \\ -H & B & -F \\ -G & -F & C \end{pmatrix}$$

then the representation of the inertia ellipsoid as bilinear form in this tensor is

$$((Tv),v) - \left(\begin{pmatrix} A & -H & -G \\ -H & B & -F \\ -G & -F & C \end{pmatrix} v,v \right) = \text{const}$$

where (a,b) is the dot product of a and b.

i.e.

$$\text{Const} = Ax^2 + By^2 + Cz^2 - 2Hxy - 2Gxz - 2Fyz$$

This ellipsoid may be thought of as the best ellipsoidal representation of the input masses. The largest eigenvalue of the tensor, T, corresponds to the narrowest waist of the ellipsoid. In the space of the eigenvectors (i.e., with the principal axes of the ellipsoid along the coordinate axes, and T in the diagonal form), the largest eigenvalue is the largest of the three sums $\sum(x^2+y^2)$, $\sum(x^2+z^2)$, $\sum(y^2+z^2)$, and it thus corresponds to the shortest principal axis. Its eigenvector is normal to the best plane in the least squares sense. Another way to view this is that the normal is the worst least squares line; this is because the sum of the squares of the distances of the points input from the normal is the largest of the three sums above.

Use: If the crystal is photographed, the views in the photo can be traced onto graph paper. Then the coordinates need only to be read off the graph paper. Appropriate scale factors can be determined by measuring the crystal. Note that the photos need not be from orthogonal directions.
On the PDP 11/40: Switch 1 turns off the VG dials
Switch 2 turns on the rotation

References:

[1] C. Scheringer, Acta Cryst., B27, 1470-72 (1971).

[2] S. D. Conte and C. de Boor, Elementary Numerical Analysis, 2nd Ed., McGraw Hill, N. Y., 1972, p. 177.

NAME: FLINUS AUTHOR: L. Andrews

CORE: 55K or 37K + Matrix (whichever is larger) DATE: October 1975

Matrix = $(nv^2+nv)/2$

Note: CM parameter must be specified on the job card.

PRØGRAM FLINUS(DATA,FØUR,PUNCH,INPUT,ØUTPUT,TINY,SHØRT,TAPE20=FØUR,TAPE14=DATA, TAPE5=INPUT,TAPE6=ØUTPUT,TAPE21=TINY,TAPE22=SHØRT,TAPE19=TAPE20)

I. PURPOSE:

Full matrix least squares refinement of crystal structures.

II. TAPES:

A. DATA-Binary or coded. Contents-ISENT,FH,FK,FL,SIG,
Purpose-data input SCALE,(E(I),I=1,25)
This file WILL be rewound.

B. FØUR-Binary Purpose-output Contents-IH,IK,IL,SINT/L,FØ,FC,
CØ,SI,DEL,SIGMA,EXTINC

FILE 1. ØRFFE (FREDFUN) file (parameters,
parameter selection
variance-covariance matrix)

FILE 2. Fourier FILE (input to JIMDAP, LIST, etc.)

III. LIMITATIONS:

	DIMENSION
A. NV-number of variables	270
B. NP-number of parameters	558
C. NA-number of atoms	50
D. NQ-number of scale factors	5
E. NS-number of symmetry cards	24
F. NF-number of form factors	15

IV. REPLACEABLE SUBROUTINES:

	ARGUMENT
A. WEIGHT-weighting	FH,FK,FL,F,SIG,SCALE,E1,E2,NREJ
B. ACCABS-reject structure factors	FH,FK,FL,F,SIG,FC,NREJ
C. CØNV-convergence	WRL,NCØN,WR
D. PATCH-special positions	I,TJ,HJ,HHJ
E. RESETX-constraints	X,Y,Z
F. RESETB-constraints	X,Y,Z
G. RESETE-constraints	EC
H. EPATCH-set symmetry constraints on extinction	EFPIP
I. NSHIFT-sets limits on change of parameters	PNEW,PØLD,DELTA,I
J. CARDIN-reads card input	ISENT,FH,FK,FL,F,SIG,SCALE,EFPIP
K. TAPEIN-reads tape input	LD,ISENT,FH,FK,FL,F,SIG,SCALE,EFPIP

V. DECK SET UP

A. JOB CARD

1. TIME LIMIT - variable
2. FIELD LENGTH - 37K + $(nv^2+nv)/2$ or 55K, whichever is larger
3. LINE LIMIT - variable
4. NUMBER OF TAPES - 0-2
5. ECS - none

B. CONTROL CARDS (NOTE: Cards marked (*) are needed only if using subroutines.)

```
*FTN(SYSEDIT)
 ATTACH(FLINUS,FLINUS,ID=CPRØGS)
 REQUEST(DATA,,,_____)          (If input on tape.)
 REQUEST(FØUR,,,_____)          (If output on tape.)
 REWIND,LGØ.
 CØPYL(FLINUS,LGØ,FLIN)
 RETURN(LGØ,FLINUS)
 FLIN.
```

If no subroutines, no saving files, minimum control cards are

```
 ATTACH(FLINUS,FLINUS,ID=CPRØGS)
 REQUEST(DATA,,,_____)
 FLINUS.
```

C. DATA CARDS:

CARD	FØRMAT
1. Title card	8A10
2. Control card 1	24I3
3. Control card 2	10I3,5F10.5
4. X-ray scattering factors	8F9.3 (4 cards per table)
5. Symmetry cards	3(F15.10,3I3)
6. Cell parameters	6F9.6
7. Parameter cards	
Scale	8F9.6
Overall temp.	F9.6
Atomic position	A6,3X,5F9.6 (for <u>each</u> atom)
Temperature parameters	6F9.6 or 6F25.6 if using commas for <u>each</u> atom)
Extinction parameter	6E12.5
8. Temperature parameter selection	72I1
9. Data (if on cards)	I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3
10. Parameter selection	72I1

D. SUMMARY FILES:

A. TINY - minimum necessary information, R factors, max shifts.
B. SHØRT - list of input, large shifts.

For fixed atom contribution these are the control cards:

```
 FTN(SYSEDIT)
 ATTACH(FLINUS,FLINUS,ID=CPRØGS)
 REQUEST(DATA,,,_____)
 REWIND(LGØ)
 CØPYL(FLINUS,LGØ,FLIN)
 RETURN(LGØ,FLINUS)
 FLIN(,FIXED)
 RETURN(FLIN,DATA)
 REWIND(FIXED)
*FTN(SYSEDIT)
 REQUEST(FØUR,,,_____)
 ATTACH(FLINUS,FLINUS,ID=CPRØGS)
*CØPYL(FLINUS,LGØ,FLIN)
*RETURN(LGØ,FLINUS)
 FLIN(FIXED)
```

*Only needed if some subroutines need to be changed in the second execution. Remember that you may have changed the weights in the first run, and you probably don't want to change them again, and if you eliminated reflections, they are not available on file FIXED.

Brookhaven Crystallographic Computer Programs

Purpose: These programs carry out full-matrix least-squares refinement of crystal structures. FLINUS is the standard version for teletype use (50 atoms maximum; 270 variables) and FLIN80 is a special version which will take up to 80 atoms but which is limited to 262 variables. For further general information on the method of this program, the user may refer to the Busing-Levy-Martin writeup of the program ØRFLS.

Input data:

I. Title FORMAT(8A10)

II. Control card FØRMAT(24I3)

1.	cols	1-3	NC	= number of cycles. = 0 for a single structure factor calculation.
2.	cols	4-6	NV	= number of parameters varied. Must be zero if NC = 0.
3.	cols	7-9	ICØNV	= 0 for no convergence test. = 1 if a convergence test (see below) is applied.
4.	cols	10-12	ICØRR	= 0 if complete correlation matrix is printed out. ≠ 0 if only correlation coefficients with $\|p\| > 0.50$ are printed out.
5.	cols	13-15	IW	= 0 if user-supplied standard deviations are to be used for weighting.
			IW	= 1 if all observations are given unit weight. (Note that the WEIGHT routine described below is called in both cases.)
6.	cols	16-18		not used
7.	cols	19-21	IT	= 0 for no parameter output on cards. = 1 for parameter output on file PUNCH
8.	cols	22-24	IXFE	= 0 for normal operation. = 1 for writing output tape suitable for input to ORFFE (FREDFUN), the Busing-Levy function and error program. (Written on file FØUR)
9.	cols	25-27	IWHSØ	= 0 if scale factors applied to F_{calc} for print-out and Fourier tape. = 1 if scale factors applied to F_{obs} for print-out and Fourier tape. Refinement is not affected by this indicator. If IWHSØ=1 then F_{obs}(printed) = F_{obs}(input tape)/Scale (input) Note that the extinction term is applied with the Scale factor.

10. cols 28-30 IWHET = -1 for a new data tape written on file FØUR with A_{calc} and B_{calc} in EFPIP(10) and EFPIP(11) for later use in fixed atom contribution mode. CAUTIØN: list on tape is ISENT,FH,FK,FL,F,SIG, SCALE,(E(I),I=1,25) and any modifications made in these quantities by SUBRØUTINE WEIGHT will be perpetuated.
= 0 for no extra tape
= 1 for normal Fourier input tape written on file FØUR

11. cols 31-33 IWHRT = 0 reflection data from cards, uses CARDIN described below. A tape or disk file is written.

= 1 reflection data from file DATA read by SUBRØUTINE TAPEIN.

12. cols 34-36 IWHTF = 0 program will stop if non-real temperature factors encountered.
= 1 program will not stop, but diagnostics will be printed out.

13. cols 37-39 IWBCD = 0 structure factors printed out on every cycle.
= -1 no print-out of structure factors.
= 1 structure factors printed out preceding first and following last cycle only.
This does not affect the FØUR tape which, if requested, is always written once and once only following the last structure factor calculation.

14. cols 40-42 IWHPS = number of sets of starting parameters.
= 0 or 1 for normal operation.
= greater than 1, the refinement will be repeated for IWHPS different sets of initial parameters. In this case, the parameter selection cards for the first cycle must be followed by new parameter cards, new parameter selection cards, new parameter cards, etc. (See below). NC cycles will be carried out for each set, and the number of parameters varied must be the same for each set.

15. cols 43-45 IWHPK = 0 for normal operation.
= 1 if a separate parameter selection card is supplied for each of the NC cycles. The parameter selection card for the first cycle must be followed by a card specifying the values of NV, NØDIV, and NØMAT for the following cycle, new parameter selection cards, etc. (See page 9.)

(Note: that IWHPS and IWHPK should not both be non-zero. Note also that IWHPK cannot be used to change from isotropic to anisotropic refinement.)

16. cols 46-48 NØDIV = 0 Normal calculation of derivatives.
= 1 Derivatives are not calculated but are taken from a FØUR file written on previous cycle.

17. cols 49-51 NØMAT = 0 for normal operation.
= 1 if inverse matrix is not calculated but is taken from FØUR file written on previous cycle.
The program will set NØMAT to 0 if NØDIV is 0

18. cols 52-54, 55-57 MANY1, MANY2
IMUCH = 1000*MANY1 + MANY2
Only the first IMUCH reflections will be used in the structure factor calculation and refinement.

19. cols 55-57 See entry immediately above.

20. cols 58-60 ITCH = 0 for normal operation.
=19 if derivatives and matrix are to be written on FØUR for later use.
Any other integer will act as 0.

21. cols 61-63 IFIX = 0 normally
= 1 for fixed atom contributions: EFPIP(10) and EFPIP(11) are added to A_{calc} and B_{calc} respectively.

22. cols 64-66 IDØVES $|\Delta F|/\sigma(F)$ default is 10. Reflections with ratios above this will be printed on file SHØRT.

23. cols 66-69 NUTS Δ/σ For parameters - parameters with Δ/σ above this value will be printed on SHØRT file if you use 0, all variable parameters are printed.

III. Control Card 2 FØRMAT(10I3,F10.5)

1. cols 1-3 IFSQ = 1 for refinement on F
= 2 for refinement on F^2
Note - the program will not transform the input quantities and it is the user's responsibility to supply F or F^2 as appropriate.

2. cols 4-6 not used.

3. cols 7-9 NF The number of x-ray form factor tables. NF should be zero for neutron diffraction. NF must include number of extra tables included to account for anomalous dispersion: see below. If NF is negative, the scattering factors are read one per card, one card per scattering factor, up to ABS(NF) cards. The latter option is included to handle neutron scattering factors (not X-ray) from these cards so anomalous scattering can be included. (untested, Feb. 1976)

4. cols 10-12 NA The number of atoms in the atoms list.

5. cols 13-15 ICENT = 1 for centrosymmetric structures with origin at center.
= 2 for all other structures.

6. cols 16-18 NS Number of symmetry cards. NS is the general space-group multiplicity in the acentric case and is equal to half this number if ICENT=1.

Note that it is not always necessary to include symmetry operations which specify lattice centering but if the user is incorporating corrections for anomalous dispersion then he has need for caution here. In particular, if the non-lattice centering symmetry operations involve non-centrosymmetric translations e.g. 1/4, 1/3, etc. such that $1/4 \neq -1/4$ as a fractional coordinate (whereas $1/2 = -1/2$ in this context) then the lattice centering operations must be included.

7. cols 19-21 NQ The number of scale factors in the parameter list.

8. cols 22-24 NAS The number of atoms for which anomalous scattering tables are provided. This is not just the number of tables but the total number of such atoms in the asymmetric unit. Note the "anomalous atoms" must be stacked in the input stream ahead of the normal scatterers.

9. cols 25-27 not used

10. cols 28-30 JEXT = 0 no extinction correction
= 1 isotropic extinction correction
= 2 anisotropic extinction correction Type I crystal
= 3 anisotropic extinction correction Type II crystal
= -2 or -3 isotropic converted to anisotropic

cols 31-40	FLAME	λ for scale factor 1	F10.5
cols 41-50	LAMBDA(2)	λ for scale factor 2	F10.5
cols 50-60	:	λ for scale factor 3	F10.5
cols 61-70	:	λ for scale factor 4	F10.5
cols 71-80	LAMBDA(5)	λ for scale factor 5	F10.5

This allows extinction to be calculated properly for different wavelengths.

IV. Scattering factor tables FØRMAT(8F9.3) or (F9.3)

Four cards are provided for each of NF tables. These are the scattering factors in order $\sin\theta/\lambda = 0.00$ [0.05] 1.55, a total of 32 numbers. These tables are omitted if NF = 0 (for neutron diffraction problems). IF anomalous scattering is to be taken care of, three sets of cards must be provided for each type of anomalous scatterer, e.g.

Set 1. f^o for anomalous scatterer 1
Set 2. $\Delta f'$ for anomalous scatterer 1
Set 3. $\Delta f''$ for anomalous scatterer 1
Set 4. f^o for anomalous scatterer 2
Set 5 and 6. $\Delta f'$ and $\Delta f''$ for anomalous scatterer 2.
etc. concluding with one set each for the normal scatterers.
Form factors for anomalous scatterers <u>must</u> come first.

If NF is negative, then neutron scattering factors are read (ABS(NF) of them), in F9.3 format.

V. Symmetry cards FØRMAT(3(F15.10.313)) NS cards.

The transformed x', y', z' are assumed to be given by the following expressions:

$$x' = t_x + I_1x + I_2y + I_3z$$

$$y' = t_y + J_1x + J_2y + J_3z$$

$$z' = t_z + M_1x + M_2y + M_3z$$

The card is then punched

cols	1-15	t_x
cols	16-18, 19-21, 22-24	I_1, I_2, I_3
cols	25-39	t_y
cols	40-42, 43-45, 46-48	J_1, J_2, J_3
cols	49-63	t_z
cols	64-66, 67-69, 70-72	M_1, M_2, M_3

If ICENT = 1 do not include cards for positions related by the center of symmetry.

VI. Cell constants FØRMAT(6F9.6)

cols 1-9	a* in reciprocal Angstroms	OR	a in Angstroms	
cols 10-18	b*	"	b	
cols 19-27	c*	"	c	
cols 28-36	cosα* or α* in degrees	"	cosα or α	in degrees
cols 37-45	cosβ* or β* "	"	cosβ or β	"
cols 46-54	cosγ* or γ* "	"	cosγ or γ	"

No indicator is necessary to specify which type of cell parameters are on this card.

VII. Parameter Cards

A. Scale factor cards FØRMAT (8F9.6). As many cards as necessary for NQ scale factors. The scale factor multiplies F_{calc} or divides F_{obs} on output depending on IWHSØ. Use the "F" scale factor for refinement on either F or F^2.

B. Overall temperature parameter F9.6. This will be added to all temperature factors.

C. Atom parameter cards for all atoms. Two cards as follows for each atom.

Card 1. FØRMAT(A6,3X,5F9.6)

cols 1-6 Any six Hollerith characters to identify the atom.

cols 7-9 Blank

cols 10-18 X-ray scattering factor number (or neutron number if NF < 0). The number of the scattering factor table containing f^o, i.e., the non-dispersive part of the form factor. This is of course the number of the only table for nondispersive scatters. It is a real number and so a decimal point should be included here. N*O*T*E--anomalously scattering atoms must be the first ones. If NF = 0, this field contains the neutron scattering factor itself.

cols 19-27 A multiplier applied to the scattering factor. This will usually be 1.0, unless symmetry conditions dictate otherwise. It may also be looked upon as a partial occupancy factor.

cols 28-36 x
cols 37-45 y
cols 46-54 z
} Fractional coordinates for this atom.

Card 2. FØRMAT(6F9.6) (if you use input separated by commas, format is 6F25.6) (Don't worry, the six 25 col. fields can be read from the one card.)

cols 1-9 B , the isotropic temperature parameter, if this is to be input. β_{11}, if anisotropic temperature parameters are input.

cols 10-18, 19-27, 28-36, 37-45, 46-54 β_{22}, β_{33}, β_{12}, β_{13}, β_{23}.

Isotropic temperature factor for atom i is defined by $\exp(-B \sin^2\theta/\lambda^2)$.

Anisotropic temperature factor expression is defined by

$$\exp(-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + 2\beta_{12}hk + 2\beta_{13}h\ell + 2\beta_{23}k\ell))$$

D. FØRMAT(6E12.5) Extinction parameters.

cols 1-12 Isotropic g or g_{11}

cols 13-24, 25-36, 27-48, 49-60, 61-72 g_{22}, g_{33}, g_{12}, g_{13}, g_{23} as defined by Coppens and Hamilton, Acta Cryst. A26, 71 (1970).

use blank if no correction

VIII. Temperature parameter selection card. FØRMAT(80I1)
Temperature parameter selection integers for each of the non-group atoms.

1 for isotropic temperature parameter
2 for anisotropic temperature parameter
3 for isotropic to be converted to anisotropic before refining
(if the 2nd or 3rd field on the TF card is non-zero, it won't be converted)

IX. Reflection data entered on cards at this point if IWHRT = 0.

The cards are read by a subroutine CARDIN (see below), and the FØRMAT is controlled by this subroutine.

ISENT = 0 except for a final card (not included in the calculation) for which ISENT = 1.

H,K,L = indices of the reflection (floating point).

FSQ = observed F^2 or F magnitude.

SIG = standard deviation assigned to this observation.

SCALE = scale factor <u>number</u> (floating point).

E(1), E(2), E(3), E(4) -- extra floating point inputs.

In FLINUS and FLIN80, up to 25 E(I) fields are available. The first seven of these must contain the following information if extinction is to be refined:

E(1), E(2), E(3) Components of the vector normal to the plane containing the incident and diffracted beams. These are components of a unit vector defined with respect to unit triclinic axes parallel to the real crystal axes. Thus, if the vector is denoted by N, we have

$$N' \begin{pmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{pmatrix} N = 1$$

E(4), E(5), E(6) Components of the vector lying in the plane of the incident and diffracted beams which is perpendicular to the incident beam. The normalization is the same as for the first vector.

E(7) TBAR, the mean path length in the crystal for this reflection, appropriately corrected for absorption as suggested by Zachariasen and as treated by Coppens and Hamilton

$$E(7) = \overline{T} = \langle te^{-\mu t} \rangle$$

where t is the path length. This is presently approximated in both BNLABS and ABSØR by

$$\overline{T} = -\frac{\ell nA}{\mu}$$

where A is the absorption.

X. Parameter selection cards. (FORMAT(72I1)

Punch 1 in column if corresponding parameter is to be varied.
Punch 0 in column if corresponding parameter is not to be varied.
The parameters are ordered as follows:

NQ scale factors.
Overall temperature parameter.
Atomic parameters.
Extinction parameters.

There are either 6 or 11 parameters.
If all atoms are isotropic, these parameters are

1. Scattering factor number.
2. Atom multiplier.
3,4,5. x,y,z
6. B.

If <u>any</u> atom is anisotropic, there are eleven parameters for each atom; for the anisotropic atoms, parameters 6-11 are β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}. For isotropic atoms parameter 6 is B, and parameters 7-11 on the parameter selection cards must contain zeros.

<u>NOTE</u>: These cards can be tedious to punch. Any card may be terminated by $ and the selection flags continued on the next card. Comments may then be punched following $ e.g.

```
11$ 2 SCALE FACTØRS
0$ ØVERALL TEMP. PARAMETER
001011$ ATØM A  INVARIANT Y
001111$ ATØM B
101111$ ATØM C
0$ ISØ.  EXT
```

THIS IS NORMALLY THE END OF THE DATA DECK. However, if either IWHPS or IWHPK is non-zero, more cards must follow.

IWHPK non-zero:

XI. FORMAT(3I3) NV, NØDIV, NØMAT for second cycle.

X. Parameter selection cards for second cycle.

XI. NV, NØDIV, NØMAT for third cycle.

.

.

.

Continue until there is a total of NC sets of parameter selection cards.

IWHPS non-zero:

VII. New parameter cards, for second parameter set.

X. New parameter selection cards, for second parameter set. (At this point, a sequence of XI and X cards may follow if IWHPK is non-zero).

VII. New parameter cards, for third parameter set.

X. New parameter selection cards for third parameter set (Type XI and X cards if IWHPK is non-zero)

Continue until IWHPS sets of parameters have been provided.

Extinction refinement in LINUS

Extinction may be refined either isotropically or anisotropically. The extinction correction, which multiplies the otherwise unmodified F_{calc}^2, is defined as

$$E = \frac{1}{\left(1 + \frac{\bar{T}\,\rho F^2\,g}{V\,\sin 2\theta}\right)^{\frac{1}{2}}}$$

where E is the printed correction term, g is the refined parameter, and

where $\rho = 2.0$ for neutron diffraction

$\rho = 2.0\ (1. + \cos^4 2\theta)\ /\ (1. + \cos^2 2\theta)$ for unpolarized X-rays.

F^2 is the calculated squared structure factor on an absolute scale. g is the extinction parameter which may be constant for all reflections or derived from an anisotropic tensor as described below.

$\bar{T}$ is the average path length in the crystal for this reflection. It is appropriately modified for absorption, as indicated above on p. 8.

$V = (V_{cell}^2/\lambda^3) \times 10^{-4}$ for neutrons if the scattering lengths are expressed in 10^{-12} cm.

$V = (V_{cell}^2/\lambda^3) \times 10^{-4} \times 12.593$ for X-rays if the scattering lengths are expressed in electrons.

The quantity 12.593 is $(mc^2/e^2)^2$.

The wave lengths are always in 10^{-8} cm.

Note that the number printed out to the extreme right on the structure-factor list is always E (the extinction correction for F^2), regardless of whether the refinement is on F^2 or F. Note also that in the printed output E is applied to either F_{obs} or F_{calc} in the same way that the scale factor is applied--depending on the value of IWHSØ (see p 1).

Interpretation of the extinction parameter g

Isotropic extinction

For isotropic extinction, we refine the parameter g as defined above. It is stored as the first extinction parameter, EC(1) or G11. It may be interpreted as follows:

Type 1 crystal (extinction dominated by mosaic spread):

η (rms mosaic spread in seconds) = 5.8186/g (see below)*

Type 2 crystal (extinction dominated by particle size).

$\bar{r}$ (radius of mean particle) = $g\lambda \times 10^{-4}$ cm

(λ in cm^{-8} and g as defined above)

Anisotropic for Type I crystal

The mosaic spread is given by a three-dimensional Gaussian described by a tensor G_{ij}:

$$g = (N'GN)^{\frac{1}{2}}$$

where N is a unit vector with components N_i relative to axes of unit length which are parallel to the real crystal axes. The vector N is described on page 7.

We may diagnonalize the tensor G in a space with metric

$$H = \begin{pmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{pmatrix}$$

to reduce it to a principal axis system. The diagonal elements may then be interpreted as follows:

η (rms in direction i) = 5.8186/SQRT(G_{ii})

---

* $5.8186 \times 10^4 = \dfrac{\text{number of seconds in 1 radian}}{2\sqrt{\pi}}$

Anisotropic for Type II crystal

The particle shape is ellipsoidal and described by a tensor G_{ij}.

$$g = (N'BN)^{-\frac{1}{2}}$$

where N is a unit vector in the plane of the incident and diffracted beams and perpendicular to the incident beam. The components are expressed relative to axes of unit length which are parallel to the real crystallographic axes.

Again we may diagonalize the tensor G in a space with metric H to obtain the principal axes of the mean particle shape ellipsoid. These may be interpreted as follows:

$$\bar{r} \text{ (in direction i)} = 10^{-4} \times \lambda/\mathrm{SQRT}(G_{ii}) \quad .$$

Reliability indices

The R-factors produced are the standard crystallographic terms--they are defined by

$$R = \frac{\sum |F_o - kF_c|}{\sum |F_o|}$$

$$wR = \left\{ \frac{\sum [w(F_o - kF_c)]^2}{\sum wF_o^{\,2}} \right\}^{\frac{1}{2}}$$

$$S = \left\{ \frac{\sum [w(F_o - kF_c)]^2}{N_o - N_v} \right\}^{\frac{1}{2}} \quad .$$

Note that in all of these expressions F_o, F_c and k may be synonymous with F_o^2, F_c^2 and k^2 respectively if the user is refining against the F_o^2's. Note also that negative F_o^2's enter into these calculations exactly as shown.

Subroutines

The following subroutines may be tailored to fit any user's particular needs.

WEIGHT

SUBROUTINE WEIGHT(FH,FK,FL,F,SIG,SCALE,E1,E2,NREJ)

E1 is dimensioned 25.

This subroutine is called after each reflection is read on each cycle. It may be used to change any of its arguments. If NREJ is set non-zero, the reflection is completely omitted from the calculation.

The dummy routine supplied sets NREJ = 0,but does nothing else.
NREJ #0 for rejection

```
      SUBROUTINE WEIGHT (H1,H2,H3,F,SIG,SCALE,E1,E2,NREJ)
      DATA ID /6HWEIGHT/
      IF (ID .NE. 0) CALL FIRST(ID)
      NREJ = 0
      RETURN
      END
```

ACCABS

SUBROUTINE ACCABS(FH,FK,FL,F,SIG,FC,NRJT)

This subroutine is called following the calculation of structure factor for each reflection. It may be used to reject structure factors from the least squares refinement or list by conditions on FC (the calculated structure factor). Set NRJT = 1 for rejection; otherwise set NRJT = 0). Note that it is quite easy to violate the principles of least squares by overly liberal use of the subroutine.

```
      SUBROUTINE ACCABS (H1,H2,H3,F,SIG,FC,NRJT)
C----INSERTED BY R.THOMAS AND P.COPPENS, 1968--ALSO KNOWN AS THE
C     SPANISH ACCABS IN HONOR OF I.BERNAL (COURTESY OF S.J.LA PLACA)
      DATA ID /6HACCABS/
      IF (ID .NE. 0) CALL FIRST(ID)
      RETURN
      END
```

CØNV

SUBRØUTINE CØNV(WRL,NCØNV,WR)

This routine is called at the completion of every structure factor calculation following a least squares cycle. WRL is the weighted R factor prior to the refinement cycle, WR is the weighted R factor following the refinement cycle. The subroutine must return to the main routine with NCØNV = 1,2, or 3.

If NCØNV = 1, the refinement continues in a normal way.
If NCØNV = 2, the main program will assume that convergence has been achieved, and the program will terminate after putting out correlation matrix and taking care of any tapes.
If NCØNV = 3, the main program will assume that the refinement has diverged, and the program will terminate after taking care of tapes. The correlation matrix is not put out, and an ØRFFE tape is not written if it was requested.

The routine supplied sets NCØNV = 3 if the weighted R factor increases by 10% and sets NCØNV = 2 if the weighted R factor changes by no more than 1/10%. THIS RØUTINE IS CALLED ØNLY IF Cols 7-9 of card 2 are non-zero.

```
      SUBROUTINE CONV (WRL,NCONV,WR)
      GOO=WR/WRL
      IF (GOO-1.10) 1050,1050,1250
1050  IF (GOO-0.999) 1200,1150,1100
1100  IF (GOO-1.001) 1150,1150,1200
1150  NCONV=2
      RETURN
1200  NCONV=1
      RETURN
1250  NCONV=3
      RETURN
      END
```

PATCH

SUBRØUTINE PATCH(I,TJ,HJ,HHJ)

This subroutine is necessary for refinement of atoms in some special positions. In the calculation of one structure factor, this routine will be called NA times for each of the NS symmetry positions. On each entry, the argument I defines the atom which is being considered so that I=1,2,...,NA on successive entries for a given symmetry position. The remaining arguments represent the transformed indices and index products. On the first entry for each symmetry position, that is, for I=1, these arguments will have been set by the program according to the information on one symmetry card. It is the task of this subroutine to modify these quantities appropriately for special position. ON SUCCESSIVE ENTRIES FOR THE SAME SYMMETRY POSITION THESE ARGUMENTS WILL RETAIN THE VALUES SET PREVIOUSLY BY THIS SUBRØUTINE. THE MAIN PROGRAM DOES NOT RESET THEM UNTIL IT ADVANCES TO A NEW SYMMETRY POSITION. The array HHJ is irrelevant when isotropic temperature factors are used, so that no difficulty will be incurred by including a subroutine prepared for the anisotropic case in an isotropic refinement. The statements required may be outlined as follows:

```
SUBRØUTINE PATCH(I,TJ,HJ,HHJ)
DIMENSION HJ(3), HHJ(6)
.
.
Interrogate I with one or more IF statements to determine
whether the values of the arguments are to be modified.
Set the values of the arguments appropriately.
.
.

RETURN
END
```

The dummy routine supplied does nothing but print out a message on first entry.

```
      SUBROUTINE PATCH (I,TJ,HJ,HHJ)
C---- DIMENSION HJ(3), HHJ(6)
      DATA ID/5HPATCH/
      IF (ID .NE. 0) CALL FIRST(ID)
      RETURN
      END
```

RESETX

SUBRØUTINE RESETX(XYZ)

This subroutine is called once near the end of each cycle of least squares. It is entered after the main output of the adjusted parameters but before the auxillary output on cards or tape. The array XYZ contains the atomic coordinates. The statements to be included are

```
SUBRØUTINE RESETX(XYZ)
DIMENSIØN XYZ(3,80)


Set the values of the constrained coordinates
equal to the appropriate functions of the parameters
which have been refined.

RETURN
END
```

The dummy routines supplied does nothing but print out a message on first entry.

```
      SUBROUTINE RESETX (XYZ)
      DATA ID /6HRESETX/
      IF (ID .NE. 0) CALL FIRST(ID)
      RETURN
      END
```

RESETB

SUBRØUTINE RESETB(BETA)

This subroutine is called once near the end of each cycle. It is entered after the main output of the adjusted parameters but before the test for positive-definite form and before the auxillary output on cards or tape. The statements to be included are as follows:

```
SUBRØUTINE RESETB(BETA)
DIMENSIØN BETA(6,80)

Set the values of the constrained parameters equal
to the appropriate functions of those which have been
refined.

RETURN
END
```

The dummy routine supplied does nothing but print out a message on first entry.

```
      SUBROUTINE RESETB (BETA)
      DATA ID /6HRESETB/
      IF (ID .NE. 0) CALL FIRST(ID)
      RETURN
      END
```

RESETE

SUBRØUTINE RESETE(EC)

This subroutine is called once near the end of each cycle of least squares. It is entered after the main output of the adjusted parameters but before the test for positive-definite form and before the output on cards and tape. It is used in case the extinction parameters have been constrained. The statements to be included are as follows:

```
SUBRØUTINE RESETE(EC)
DIMENSIØN EC(6)

Set the values of the constrained parameters
equal to the appropriate functions of those
that have been refined.

RETURN
END
```

The dummy subroutine supplied does nothing but print out a message on first entry

```
SUBROUTINE RESETE (EC)
DATA ID /6HRESETE/
IF (ID .NE. 0) CALL FIRST(ID)
RETURN
END
```

EPATCH

SUBRØUTINE EPATCH(EFPIP)

This subroutine is called only if extinction is anisotropic. It may may be used to set symmetry or other constraints on refinement of the extinction parameters. For example, in a tetragonal crystal we may wish to constrain $g_{11} = g_{22}$, $g_{13} = g_{23} = g_{12} = 0$.

An appropriate patch might be as follows:

```
      SUBRØUTINE EPATCH(EFPIP)
      DIMENSIØN EFPIP(25)
      EFPIP(1) = SQRT(EFPIP(1)**2 + EFPIP(2)**2)
      EFPIP(2) = 0.0

C     THIS FIXES THINGS UP FOR TYPE 1 EXTINCTION.
C     WE WOULD REFINE ONLY G11 and G33

      EFPIP(4) = SQRT(EFPIP(4)**2 + EFPIP(5)**2)

      EFPIP(5) = 0.0

C     THIS FIXES UP IN SIMILAR WAY FOR TYPE 2 EXTINCTION

      RETURN
      END
```

The subroutine could also be used to calculate the appropriate vectors in EFPIP if this had not been done by the processor.

The dummy subroutine supplied does nothing but print out a message on first entry.

```
      SUBROUTINE EPATCH (EFPIP)
      DATA ID/6HEPATCH/
      IF (ID .NE. 0) CALL FIRST(ID)
      RETURN
      END
```

NSHIFT

SUBRØUTINE NSHIFT(PNEW,PØLD,DELTA,I)

This subroutine is entered after the least squares refinement as each parameter I is being corrected. PØLD is the value of the parameter prior to the cycle, DELTA is the shift, and PNEW = PØLD + DELTA is the new value of the parameter. The routine may be used to change PNEW usually to aid in the convergence. The routine supplied modifies the extinction parameters in a way which aids convergence when the starting values are far from the correct ones. This part of the routine should not be changed. Partial shifts may be applied to other parameters, if desired, by rewriting the routine such that instead of the statement.

```
IF(IFFLAG .EQ. 0) RETURN
```

a statement

```
IF(IFLAG .EQ. 0) GO TO 1

................

1 statements to apply partial shifts to other than
extinction parameters, GO TO 1150 if a partial shift
is applied, otherwise:

RETURN
END
```

Note that if this routine is replaced, you don't need to include commons.

```
      SUBROUTINE NSHIFT (PNEW,POLD,DELTA,I)
      COMMON /DERIV/ DADX,DADB,DBDX,DBDB,DADAI,DADFI,DBDAI,
     2  DBDFI,DFDC,DFDS,DFDTO,DC,DY
      COMMON /REAL/ A,AI,ATOM,B,BETA,BLANKS,EC,EFPIP,EXTINC,F,FS,FX,HJ,H
     1HJ,DIAG,LAMBDA,P,PHVOL,PD,PRCP,RCP,ROW,SC,SF,SIG,SIGYO,SINTHL,SMOO
     2M,SQRTAB,SQSIG,TFI,TITLE,TJ,TO,TS,V,VOLUME,X,XYZ,YO,DOVE,DOVES
     2,SIN2T
      COMMON /CCARD1/ NC,NV,ICONV,ICORR,IW,IP,IT,IXFE,IWHSO,IWHET,IWHRT,
     1IWHTF,IWBCD,IWHPS,IWHPK,NODIV,NOMAT,MANYR1,MANYR2,ITCH,IDOVES,NUTS
      COMMON /CCARD2/ IFSQ,ITF,NF,NA,ICENT,NS,NQ,NAS,NANISO,JEXT,FLAME
      COMMON /INTEGR/ IC,IEFLAG,IEXT,IEOF,IFFLAG,IFIX,IHKL,
     2  IMUCH,ISTEP,IWALT,JTF,KI,LABEL,NCY,NUMEXT,NM,NO,NP,NX
C----AM MUST BE DIMENSIONED AT LEAST N*(N+1)/2 TO HOLD THE MATRIX
C IN THE PAST IT HAS BEEN DIMENSIONED N*(N+3)/2
      COMMON AM(1)
      REAL LAMBDA(5)
C-----NV=270
      DIMENSION V(270), DV(270), DIAG(270), PD(270), ROW(270)
C----NP=558
      DIMENSION P(558), KI(558), DC(558)
C----NA=50
      DIMENSION ATOM(51)
      DIMENSION SF(50), AI(50), XYZ(3,50), BETA(6,50), DADFI(50), DBDFI(
     150), DADAI(50), DBDAI(50), DADX(3,50), DBDX(3,50), DADB(6,50), DBD
     2 B(6,50),JTF(50)
C----NQ=5,NS=24,NF=15
      DIMENSION SC(5), DFDS(5), TS(3,24), FS(3,3,24), FX(32,15)
      EQUIVALENCE (BLANKS,IBLANK)
      EQUIVALENCE (DC,DV)
      EQUIVALENCE (IHKL(4),IQ)
      EQUIVALENCE (IQ,IWCH)
      DIMENSION EFPIP(25), EC(6), LABEL(21), TITLE(8), X(4), SQSIG(2),
     1 IHKL(4), HJ(3), HHJ(6), RCP(6), PRCP(6)
      DIMENSION IHKL3(3)
      EQUIVALENCE (IHKL,IHKL3)
      DIMENSION DFDC(6)
      COMMON /IO/ LD,LE,LF,LI,LO,ITINY,ISHRT1,ISHRT2
      DATA ID /6HNSHIFT/
      IF (ID .NE. 0) CALL FIRST(ID)
      IF (IFFLAG .EQ. 0) RETURN
      IF (IFFLAG .GE. 4) GO TO 1200
      IF (POLD .LE. 0.0) RETURN
      IF (PNEW .LE. 0.0) GO TO 1050
      IF (ABS(DELTA) .GT. 0.5*POLD) GO TO 1100
      RETURN
 1050 PNEW=0.5*POLD
      GO TO 1150
 1100 CONTINUE
      FACTOR=1.0


      PNEW=POLD+((PNEW+POLD)/(2.0*POLD))**FACTOR*DELTA
 1150 WRITE (LO,1300)
      WRITE (ITINY,1250) I
      RETURN
 1200 IF (POLD*PNEW .LT. -0.1) GO TO 1050
      RETURN
C
C
 1250 FORMAT (25H PARTIAL SHIFT FOR PARAM.I5)
 1300 FORMAT (55H0NOTE***FULL SHIFT NOT APPLIED TO FOLLOWING PARAMETER
     1)
      END
```

CARDIN

SUBRØUTINE CARDIN(ISENT,FH,FK,FL,F,SIG,SCALE,E)

Reads in reflection data cards in a format to be specified by user. (E(I),I=1,7) have special meaning for the extinction refinement.

The use of this routine is wasteful in terms of paper, time and money. A better procedure is to produce a file, called DATA, which contains the reflections and to modify TAPEIN accordingly.

```
      SUBROUTINE CARDIN (ISENT,FH,FK,FL,F,SIG,SCALE,E)
      DIMENSION E(7)
      DIMENSION IFMT(20)
      COMMON /IO/ LD,LE,LF,LI,LO,ITINY,ISHRT1,ISHRT2
      DATA ID /6HCARDIN/
      DATA IFMT/4H(I1,,4HF3.0,4H,2F4,4H.0,2,4HF9.3,4H,F3.,4H0,7F,
     X 4H6.3),12*4H    /
      IF (ID .NE. 0) CALL FIRST(ID)
   10 READ (LI,IFMT) ISENT,FH,FK,FL,F,SIG,SCALE,E
      IF (ISENT.EQ.9) READ(LI,20) IFMT
   20 FORMAT (20A4)
      IF (ISENT.EQ.9) GO TO 10
      WRITE (LO,1050) ISENT,FH,FK,FL,F,SIG,SCALE,E
      RETURN
C
C
 1050 FORMAT (I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3)
      END
```

The routine supplied will read cards containing quantities corresponding to the formal arguments of the subroutine in FORMAT (I1,F3.0,2F4.0, 2F9.3, F3.0,7F6.3) and return these to the calling routine (PRELIM). The cards read are written to OUTPUT from CARDIN and written to the file DATA by PRELIM. The user may change the FORMAT to be used in reading his/her cards by supplying a dummy first card containing a 9 in ccl, a new FORMAT specification on the second card and following these with the reflection data.

TAPEIN

SUBRØUTINE TAPEIN(LD,ISENT,FH,FK,FL,F,SIG,SCALE,EFPIP)

Reads in the data tape. EFPIP is dimensioned for EFPIP(25). LD is the tape number supplied by the calling program. The routine supplied (listing below) will read either coded or binary input without the user having to inform it of which to expect. Two different coded formats are also permitted. The data file may be terminated with either ISENT=1 or an end-of-file. If the first data card is of the form

col 1	col 80
9	9

the next card must be the format specification starting with an open parenthesis and ending with a close parenthesis. The data will be read by

READ(LD,IFMT)ISENT,FH,FK,FL,F,SIG,SCALE,(EFPIP(IU),IU=1,8)

Data cards then follow.

```
      SUBROUTINE TAPEIN (LU,ISENT,FH,FK,FL,F,SIG,SCALE,EFPIP)
C
C     THIS VERSION OF TAPEIN FOR FLINUS READS THE BINARY INPUT RECORDS
C     AND THEN DECIDES WHETHER THE H,K,L AND SCALE VARIABLES ARE WRITTEN
C     AS INTEGERS OR FLOATING POINT .  APPROPRIATE ACTION IS TAKEN TO
C     ENSURE THAT THE H,K,L ARE  RETURNED TO THE CALLING ROUTINE AS
C      FLOATING POINT QUANTITIES.
C                                                GJB WILLIAMS  JAN/18/75
C
C
C     FURTHER REVISED TO ACCEPT THE TWO CODED FORMATS
C                                                     HJB. 18-JAN-75
C
      DIMENSION IRAY(7), FRAY(7), IRAYT(2), EFPIP(25)
      DIMENSION IFMT(20)
      EQUIVALENCE (IRAY(1),IRAYT(1))
      EQUIVALENCE (IRAY(1),FRAY(1))
      DATA MSK/77770000000000000000B/,INTG/0/,IENTER/6HTAPEIN/
      LD=LU
      IF (IENTER.EQ.0) GO TO 30
      CALL FIRST (IENTER)
      ITEST=0
      CALL INMODE (ITEST)
      IF (ITEST.GT.0.AND.ITEST.LT.5) GO TO 30
      REWIND LD
      READ (LD) IRAYT(1),IRAYT(2)
      IRR=IRAYT(2).AND.7777B
      IF (IRR.EQ.0) GO TO 10
      IF (IRR.EQ.7777B) GO TO 10
      IRR=IRAYT(2).AND.MSK
      IF (IRR.EQ.MSK.OR.IRR.EQ.0) GO TO 10
      ITEST=5
      IF(IRAY(1).EQ.1H9)GO TO 110
      ITST=IRAY(2).AND.77B
      ITEST=4
      IF (ITST.EQ.1P.) ITEST=3
      REWIND LD
      GO TO 30
```

```
   10 REWIND LD
      READ (LD) IRAY,EFPIP
      ITEST=1
      DO 20 I=2,4
      IF(IRAY(I).EQ.0)GO TO 20
      JTEST=IRAY(I).AND.MSK
      IF (JTEST.EQ.MSK.OR.JTEST.EQ.INTG) ITEST=2
   20 CONTINUE
      REWIND LD
   30 GO TO (40,40,60,70,120), ITEST
   40 READ (LD) IRAY,EFPIP
      ISENT=IRAY(1)
      F=FRAY(5)
      SIG=FRAY(6)
      IF (ITEST.GT.1) GO TO 50
      FH=FRAY(2)
      FK=FRAY(3)
      FL=FRAY(4)
      SCALE=FRAY(7)
      GO TO 80
   50 FH=IRAY(2)
      FK=IRAY(3)
      FL=IRAY(4)
      SCALE=IRAY(7)
      GO TO 80
   60 READ (LD,90) ISENT,FH,FK,FL,F,SIG,SCALE,(EFPIP(IU),IU=1,8)
      GO TO 80
   70 READ (LD,100) ISENT,FH,FK,FL,F,SIG,SCALE,(EFPIP(IU),IU=1,8)


   80 CONTINUE
      IREP=0

      IF (IREP.NE.0) GO TO 30
      RETURN
  120 READ (LD,IFMT) ISENT,FH,FK,FL,F,SIG,SCALE,(EFPIP(IU),IU=1,8)
      GO TO 80
  110 READ (LD,130) IFMT
  130 FORMAT(20A4)
      GO TO 30
C
   90 FORMAT (I1,F3.0,2F4.0,F11.3,F10.3,F3.0,6F6.3,F8.5,F5.1)
  100 FORMAT (I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3,F5.1)
      END
```

Tape and Disk Files

DATA

Contains reflection data. It may be supplied as an input tape. If input is on cards, the cards can be copied onto this file by CARDIN, but it is better to use TAPEIN for most cases.

Binary or coded file. One record per reflection.

For each reflection:

ISENT,FH,FK,FL,F,SIG,SCALE,(E(I),I=1,25)

ISENT = 0 After last reflection, a dummy reflection with ISENT=1 terminates the data input. This is supplied automatically by AVSØRT, BNLABS and CØRDAT. The DEFAULT subroutine TAPEIN will stop at EOF.

FH,FK,FL = indices of reflection.

F = F or F^2

SIG = standard deviation of F or F^2 for use in weighting.

SCALE = scale factor number (an integer) for this reflection.

E(I), I = 1, 25 are extra input at discretion of user. For refining extinction coefficient in Zachariasen approximation or for adding fixed contributions to structure factors, these fields may have special meaning.

The file is terminated by a record of the same length with ISENT = 1.

FØUR

FØUR contains input files for FREDFUN and for JIMDAP. These are separated by a single end-of-file, and will be preceded by the derivatives if these are written out.

1. The FREDFUN file consists of the parameters, parameter selection information and error matrix in the order specified in the program listing. This file is terminated by an end-of-file mark.

2. The Fourier file is written if requested on the first control card. It consists of one record per reflection as follows. It is a binary file.

   IH,IK,IL,S,FØ,FC,CØ,SI,DEL,SIGMA,SPLAT

   IH,IK,IL are fixed point indices

   S is $\sin\theta/\lambda$

   FØ is the appropriate amplitude for an observed Fourier.

   FC is the appropriate amplitude for a calculated Fourier.

   CØ is the cosine of the calculated phase angle.

   SI is the sine of the calculated phase angle.

   DEL is the appropriate amplitude for a difference Fourier.

   SIGMA is the standard deviation of the reflection.

   The quantities have been appropriately modified if anomalous dispersion is present, and FØ has been multiplied by scale and extinction factors.

   If the calculation was on F^2 rather than F, F^2 and ΔF^2 values will be written on tape.

   The Fourier file is terminated by an end-of-file mark only, not by IH = 999 as in some earlier versions of the program

   FØUR may be used for storage of derivatives and matrix between cycles. See listings for order of information. This file is written only if requested on the control card.

TINY

TINY file of output for use on teletype. Gives error messages, R factor and maximum shifts.

SHØRT

SHØRT file of least squares shifts and structure factor information for reflections with Δ/σ greater than specified by NUTS (control card 1)

Dimensions

	FLINUS	FLIN80
NV-- number of variables	270	262
NP--number of parameters	558	889
NA--number of atoms	50	80
NQ--number of scale factors	5	5
NS--number of symmetry cards	24	24
NF--number of form factors	15	15

Maximum FL for maximum NV is (150000_8)

Execution FL $(55000)_8$ or $(37000_8$ + matrix) whichever is larger.

Brookhaven Crystallographic Computer Program

NAME: FMUD1 TIME: $<17_8$ SECS

Purpose:

FMUD1 allows convenient input of setting angles and performs least-squares refinement of unit cell constants, orientation angles, and machine zeroes. The correction of ω values from the neutron spectrometers is done automatically, and default σ values are provided for setting angles.

PRØGRAM FMUD1(INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT)

Input:

Card 1 FØRMAT(9A6) (TITLE(I),I=1,9)

cols. 1-54 BCD title

Card 2 FØRMAT(4F10.0) ANGZER(4),ANGZER(1),ANGZER(2),ANGZER(3)

Machine zeroes $2\theta_0, \omega_0, \chi_0, \phi_0$. Display readings at true zero will be added to computed settings to obtain scale readings.

Card 3 FØRMAT(F10.5,3I5) FLAMB,ITECH,ICØRSW,INPSW

cols. 1-10 Wavelength in Å

11-15 ITECH=0 Setting angles from a coupled ($\theta/2\theta$) instrument (X-ray)
ITECH=1 Setting angles from an uncoupled instrument (Neutron machines)

16-20 ICØRSW set non-zero to print correlation matrix

21-25 INPSW set non-zero to print U matrix input data

Card 4 FØRMAT(3F2.0) (PLUS(K),K=1,3)

Parities of ω, χ, ϕ in Hamilton convention. See International Tables, Vol. 4, p. 276 for definitions.

-1 -1 -1 FØR H6MAIN
-1 +1 -1 FØR H6SATT
-1 -1 -1 FØR XRAY7

Cards 5 Setting angle data

(FØRMAT(3F4.0,4F9.2,3F8.2) (H(J,I),J=1,3),2THETA(I),ØMEGA(I), CHI(I),PHI(I),WAYØ(1,I),WAYØ(2,I),WAYØ(3,I). The last three quantities are $\sigma(2\theta)$,$\sigma(\chi)$,$\sigma(\phi)$. $\sigma(2\theta)$ and $\sigma(\chi)$ are preset to 0.05 and 0.08 if not specified. $\sigma(\phi)$ is set as follows

χ^{o}	$\sigma(\phi)^{o}$
0-55	0.02
55-65	0.03
60-65	0.04
65-70	0.06
70-75	0.08
75-80	0.12
80-85	0.20
85-90	1.0
90-	20.0

Reflection data to refine cell constants, orientation angles, and/or machine zeroes by least squares. 1 50 reflections maximum. (20-29 independent reflections well-distributed in reciprocal space give good results.) Program will use observed settings for first three reflections to calculate initial cell constants and orientation angles so be sure first three reflections have indices that are linearly independent.

Card 6 FØRMAT(F4.0) 999 Termination indicator

Card 7 FØRMAT(13I1) (KEY(I),I=1,13)

selection flags for refinement of a,b,c,cosα,cosβ,cosγ,

$\phi_s,\chi_s,\omega_s,\omega_0,\chi_0,\phi_0,2\theta_0$.

Here ϕ_s,χ_s,ω_s are the orientation angles defined in International Tables, vol. 4, pp 280-281.

KEY(I) = 1 parameter I is refined
= 0 parameter I is not refined

Card 8 FØRMAT(3F4.0,F9.2) ((H(I),I=1,3),ØMEGA)

h,k,ℓ list of reflections for which FMUD1 will calculate and print setting angles. ØMEGA is the offset (in degrees) from the bisecting position which the program will use in the setting angle calculation (usually ØMEGA will be zero). Terminate with h=999. The list can be omitted entirely using 1 card with h=999.

(end of input)

The following subroutine may be supplied by the user:

```
SUBRØUTINE PATCH (A,ØRT,ANGZER)
```

This is used to get parameter restrictions into the least-squares refinement. For example, if material is cubic, we set

```
A(2) = A(1)
A(3) = A(1)
```

and refine only A(1).

A(6) are cell constants

ØRT(3) are orientation angles ϕ_s, χ_s, and ω_s

i.e.,

```
SUBRØUTINE PATCH (A, ØRT, ANGZER)
DIMENSIØN A(6), ØRT(3), ANGZER(4)
.....  }
.....  }  instructions
RETURN
END
```

A dummy routine is supplied.

Output:

Output has been condensed to 58 columns to fit a teletype, and consists of the following:

1. Summary of input information and reflection data (optional).
2. Cell constants, U matrix and orientation angles initially determined from the first 3 reflections.
3. Cell constants, orientation angles and machine zeroes with standard deviations after each cycle of least-squares refinement.
4. Calculated setting angles at convergence for reflections used in the refinement, and the differences from the original reflection data. Δ = obs-calc.
5. Refined cell constants, orientation angles and U matrix; correlation matrix (optional).
6. Settings for special list of reflections, if any.

Brookhaven Crystallographic Computer Program

NAME: FREDFUN Files 3 Time Short

FL: 45K + MATRIX*

This is a slight modification of Busing-Levy ØRFFE with least-squares plane option.

```
PRØGRAM  FREDFN(FØUR,INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE12=FØUR,
    TAPE19=TAPE12,TAPE16)
```

*Sufficient field length to accommodate variance-covariance matrix

$$= \frac{NV(NV + 1)}{2}$$

Minimum FL $(45000)_8$

Maximum FL $(45000)_8 + (37000)_{10} = (156000)_8$

FREDFUN. Crystallographic function and error program.

DATA INPUT FOR FREDFUN

1. FORMAT(12A6) Title.

2. FORMAT(24I3) Control integers.

1-3 IC(1) Variance-covariance matrix will

0 not be used
1 read from tape prepared by FLINUS program.
2 read from cards

4-6 IC(2) Number of structure parameters to be read from cards. If IC(2) = 0, parameters will be read from tape.

7-9 IC(3) Cell parameter errors are

0 not to be used
1 read in the form of standard errors
2 read in the form of a variance-covariance matrix

10-12 IC(4) The number of symmetry cards to be read. Maximum 48. Minimum 0.

13-15 IC(5) Order of variance-covariance matrix if read from cards. Zero if read from tape

16-18 Irrelevant

19-21 IC(7) Period of position parameters in the parameter list if read from cards.

22-24 IC(8) Position of first position parameter in parameter list if read from cards.

25-27 IC(9) Period of temperature factor coefficients in parameter list if read from cards.

28-30 IC(10) Position of first temperature factor coefficient in parameter list if read from cards.

31-33 NF, number of files to be skipped on tape prepared by FLINUS (As of 1973 this should always be 0).

34-36 NT, number of translation cards to be read in. May be zero.

37-39 IDR = 0. Direct cell constants will be read in.

IDR = 1. Reciprocal cell constants will be read in.

3. FORMAT(8F9.4) Atomic parameters if supplied on cards. In same FORMAT as for FLINUS Scale factor and overall temperature factor cards must be supplied even if blank. Also two cards for each atom as in FLINUS.

Thus the position parameters for atom I start with P(J) where J =IC(7)*(I-1) + IC(8).

Thus the temperature factor coefficients for atom I start with P(K) where K = IC(9)*(I-1)+IC(10)

4. FORMAT(72I1) Parameter selection integers. As many cards as necessary provided only if the matrix is read from cards. Identifies those parameters which are represented in the variance-covariance matrix. Punch 1 in column I if parameter I is represented. Otherwise 0.

5. FORMAT(6E12.6) Variance-covariance matrix if read from cards.

   Card 5A. 1-12 Scale factor by which whole matrix is multiplied by the program.
   Cards 5B. N(N+1)/2 elements of variance-covariance matrix in order

   11,12,...,1N,22,23,... 2N,33,...NN

6. FORMAT (6F9.4) Cell parameters. A,B,C,COS(α),COS(β),COS(γ) if IDR = 0
   Reciprocal cell parameters in same order if IDR = 1.

7. Cell parameter errors, if requested.

   If IC(3) =1, FORMAT(6F9.4) Standard deviations on the six cell parameters.

   If IC(3) = 2 FORMAT(8F9.4) Error matrix for cell parameters

   Card 7A. AA,AB,AC,AALPHA,ABETA,AGAMMA,BB,BC
   Card 7B. BALPHA,BBETA,BGAMMA,CC,CALPHA,CBETA,CGAMMA,ALPHAALPHA
   Card 7C. ALPHABETA,ALPHAGAMMA,BETABETA,BETAGAMMA,GAMMAGAMMA

   Note that errors for <u>direct cell</u> must be provided even if reciprocal cell parameters are read in on previous card.

8. Symmetry cards. FORMAT (3 (F15.5,3I3)). See write-up of LINUS for complete description. FORMAT is identical.

9. Translation cards (Optional) 3F10.8. See SADIAN writeup for complete description.

10. Instruction cards as indicated on the following page and as discussed in more detail in the Oak Ridge publication on ORXFE (Publication Number 59-4-37)

11. Blank card.

Instruction cards for functions.

Molecule designation = 100c + s

Atom designation = 6 digit integer made up in the following way:

1000 a + 100 c + s

a is the number of the atom in the parameter list.
s is the number of the symmetry transformation to be applied. May be zero.
c defines the unit cell translations as follows. (This translation is applied after the symmetry transformation.)

NB If one wants +1 on any of the cell edges then it can be produced by subtracting 1 from "the other atom". Symmetry element number 0 is the identity transformation. It is always present (internal to the program) and need not be supplied.

c	x"	y"	z"
0	x'	y'	z'
1	x'-1	y'	z'
2	x'	y'-1	z'
3	x'-1	y'-1	z'
4	x'	y'	z'-1
5	x'-1	y'	z'-1
6	x'	y'-1	z'-1
7	x'-1	y'-1	z'-1

The function designation is always in columns 1-3, e.g., Function 376 is punched 376 in columns 1-3.

FUNCTION 001 One interatomic distance

4-9 atomic designation 1
10-15 atom designation 2

FUNCTION 101 All distances less than dmax between atoms in two molecules

4-6 Number of atoms in the parameter list
7-9 Molecule designation 1
10-12 Blank
13-15 Molecule designation 2 (May be same as 1.)
16-18 Integer 10*dmax in Angstroms. If left blank will be set to 4.0 A.

FUNCTION 201 All distances less than dmax between all atoms in the basic molecule and all molecules formed by all combinations of c,s, and t.

4-6 Number of atoms in the parameter list.
7-15 Blank
16-18 10*dmax

FUNCTION 002 2 Angle defined by three atoms

4-9 Atom designation 1
10-15 Atom designation 2 (vertex)
16-21 Atom designation 3

FUNCTION 102 Calculate all angles between atoms within one molecule if short sides < dmax.

FUNCTION 202 Same as 102 for all molecules formed by all combinations of c, s, and t.

FUNCTION 003 Dihedral angle between planes each defined by three atoms.

4-9, 10-15, 16-21 Atom designations for first plane

22-27, 28-33, 34-39 Atom designations for second plane

Note that if 10-15 and 16-21 are equal, angle is obtained between the second plane and the vector described by (4-9) ⟶ (10-15)

FUNCTION 004 Difference between two interatomic distances

4-9 , 10-15 Atom designations for distance 1.
16-21, 22-27 Atom designations for distance 2.

FUNCTION 005 Difference between two angles, each defined by three atoms

4-9 , 10-15, 16-21 atom designations for angle 1
22-27, 28-33, 34-39 atom designations for angle 2

FUNCTION 006 The sum of several angles, each defined by three atoms

4-6 Number of angles to be summed.
7-12, 13-18 19-24 Atom designations for angle 1
25-30, 31-36, 37-42 Atom designations for angle 2
etc.

FUNCTION 007 RMS component of thermal motion along principal axis r

4-9 Atom designation
10-12 r = 1,2, or 3

FUNCTION 107 Same as 007 for each of the three values of r

4-9 Atom designation

FUNCTION 207 Same as 107 for each atom of a given molecule

4-6 number of atoms in parameter list
7-9 molecule designation

FUNCTION 008 Angle between principal axis r of atom 1 and a vector defined by atoms 2 and 3.

4-9 Atom designation 1
10-12 r = 1,2, or 3
13-18 Atom designation 2
19-24 Atom designation 3

FUNCTION 108 Same as function 008 for each of the three values of r

4-9 Atom designation 1
10-12 Blank
13-18 Atom designation 2
19-24 Atom designation 3

FUNCTION 208 Same as 108 for each atom in a given molecule

4-6 Number of atoms in parameter list
7-9 Molecule designation
10-12 Blank
13-18 Atom designation 2
19-24 Atom designation 3

FUNCTION 009 RMS component of thermal motion of atom along principal axis r projected on a vector defined by atoms 2 and 3

Input same as 008.

FUNCTION 109 Same as 009 for each value of r

Input same as 108.

FUNCTION 209 Same as 109 for all atoms in a given molecule.

Input same as 208.

FUNCTION 010 Angle between principal axis r of atom 1 and axis i of a Cartesian coordinate system. The latter is defined by atoms 2, 3, 4, and 5 as follows: Axis 1 is the vector (2,3) Axis 2 is (Axis 1) X (4,5). Axis 3 is (Axis 1) X (Axis 2).

4-9 Atom designation 1
10-12 r = 1,2, or 3
13-15 i = 1,2, or 3
16-21 Atom designation 2
22-27 Atom designation 3
28-33 Atom designation 4
34-39 Atom designation 5

FUNCTION 110 Same as function 010 for the nine combinations of r and i.

Input same as 010, but columns 10-15 blank.

FUNCTION 210 Same as function 110, but for all atoms in a given molecule.

4-6 Number of atoms in parameter list
7-9 Molecule designation
16-39 As in function 010

FUNCTION 011 RMS component of atom 1 along principal axis r, projected on axis i of a Cartesian system defined by four atoms as in function 10.

Input same as function 010.

FUNCTION 111 Same as function 011, except for all combinations of r and i.

Input same as function 110.

FUNCTION 211 Same as function 111, except for all atoms in a molecule.

Input same as function 210.

FUNCTION 012 RMS component of thermal displacement of atom 1 in the direction of a vector defined by atoms 2 and 3.

4-9, 10-15, 16-21 atom designations 1, 2 and 3.

FUNCTION 013 RMS radial thermal displacement of an atom

4-9 Atom designation

FUNCTION 014 Interatomic distance corrected for "riding". The second atom "rides" on the first atom.

4-9, 10-15 atom designations

FUNCTION 015 Interatomic distance corrected for independent motion.

4-9, 10-15 atom designations

FUNCTION 016 Least squares plane (NB. FREDFUN will fail on three atom planes)

4-6 Number of atoms

7-12, 13-18, 19-24, 25-30 etc. atom designations

A maximum of twenty atoms can be handled with this function. If the matrix is input from tape, the program will not handle atoms with no errors, i.e., certain special positions or unrefined, nor will it handle atoms related by symmetry, because there is complete correlation between parameters. Although errors on coefficients of plane are meaningless, the sum-of-squares value printed out may be tested as chi-square with n-3 degrees of freedom.

For atoms in special positions or related by symmetry, the following option should be used:

Following the designation of atom numbers for atoms which are to be included in the least squares plane, sufficient fields must be provided for a weight for each atom, that is, a three column field for each atom. (I3 format) If the field for the first atom is zero or blank, the atoms are weighted according to the information obtained from the least squares variance-covariance matrix input to ORFFE. If the first field is not blank or zero then it and subsequent fields contain the weights to be assigned to the successive atoms in the least squares determination of the plane; the variance-covariance matrix from the least squares is completely ignored in this case. Thus, if one is considering ten atoms and wishes to find the plane through the first six atoms but only to determine the deviations from the plane of the last four atoms, the fields for the weights should be 1111110000. If the weights are to be determined from the least squares variance-covariance matrix the weight field should be zero for all atoms. Even in this case it is necessary to provide enough fields for weights to be assigned, using continuation cards if necessary.

N.B. FOR ALL FUNCTIONS. Only the first 23 fields on a card are to be considered part of an instruction. If a non-zero integer is punched in the 24th field (columns 70-72), the instruction is continued on the following card. Up to 10 cards may be used if necessary.

If there are constraints on the parameters, and if errors are to be computed properly, subroutines SETA and SETP must be provided.

SUBROUTINE SETA(A), DIMENSION A(6), COMMON if required
SUBROUTINE SETP(P), DIMENSION P(890), COMMON if required

Maximum number of Parameters = 890

Maximum size of matrix $(37000)_{10} = \frac{(NV \cdot (NV + 1))}{1}$

Maximum number of parameters varied NV = 270

Brookhaven Crystallographic Computer Program

Name: GENATM Time: $< 5_8$ sec

Core: 15 K_8

PRØGRAM GENATM(INPUT,ØUTPUT,PUNCH,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE7=PUNCH)

Purpose: This program was designed to determine new positions (atomic sites) given certain positions and geometric constraints. Its most common purpose is to predict hydrogen atom locations from a knowledge of the framework to which the hydrogen atoms are bonded.

This program was written by R. Shiono of the University of Pittsburgh. It was installed at BNL by L. C. Andrews and G. J. B. Williams.

Given a set of unit cell constants and a set of atomic coordinates, this program generates a new position with a given distance from an atom specified with various geometric conditions such as bond angles, torsional angles. The condition also includes the direction parallel to a specified vector or perpendicular to the specified plane.

Once any position is generated, its coordinates will be stored in the program and this new position may be used for any further generation of positions.

Generation Options

The following drawings illustrate the various options available in generating a new atomic position.

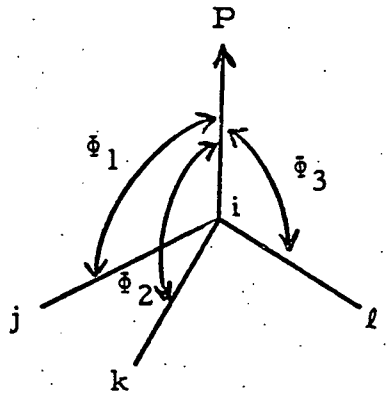


Fig. 1

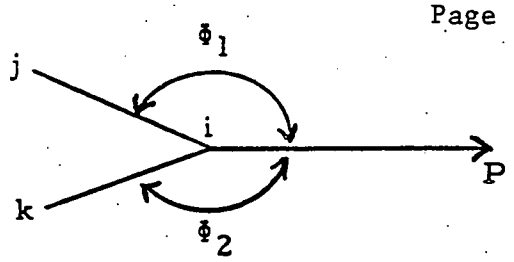


Fig. 2

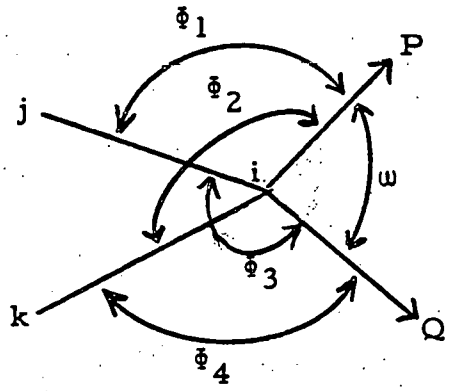


Fig. 3

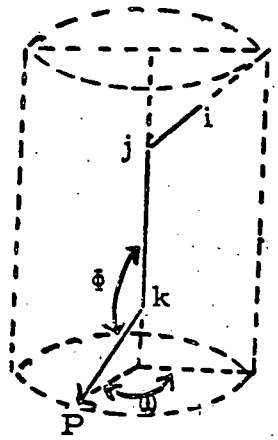


Fig. 4

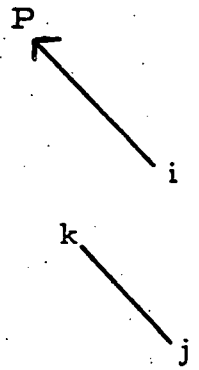


Fig. 5

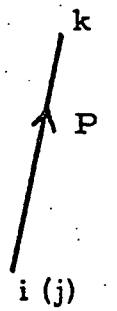


Fig. 5'

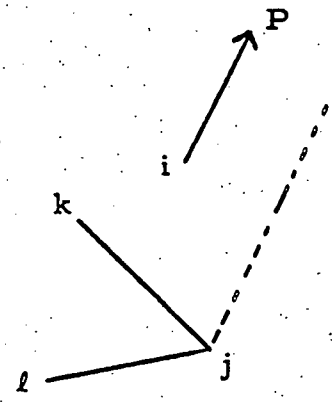


Fig. 6

Card Format:

1) Title Card (20A4)

Any alphanumeric information on a card. The contents will be reproduced on the output.

2) Unit Cell Constant Card (6F9.6)

Cols	1-9	a in Å units
	10-18	b in Å units
	19-27	c in Å units
	28-36	cosα or alpha in degrees
	37-45	cosβ or beta in degrees
	46-54	cosγ or gamma in degrees

This is the standard format for the unit cell constants.

3) Control Card (2I5)

Cols 3-5 Number of atomic coordinates to be read. The maximum number allowed currently is 150, including those atoms to be generated.

10
- 0 For the input coordinate cards, only the positional parameter cards are present.
- 1 The temperature factor cards are interspersed and to be skipped by the program in reading.
- 2 The estimated standard deviation cards are also present and to be skipped.

4) Coordinate Cards (A4,A2,21X,3F9.6)

This is the standard coordinate card format commonly used by many programs.

Cols	1-6	Any six Hollerith characters (or blank) for the identification.
	28-36	x (fractional coordinate)
	37-45	y
	46-54	z

The temperature factor and the estimated standard deviations cards may follow the positional parameter cards as in the Structure Factor program.

5) Specification Cards (5I5,3F10.3,4X,A4,A2)

Cols 4-5 This column specifies the option to be used to generate a new atomic position or two.

0 (blank) Place an atom in the direction of a line making three equal obtuse angles to the three intersecting lines at the apex. In Fig. 1, thus choose the direction with $\Phi_1 = \Phi_2 = \Phi_3$.

This requires four atomic specifications, i, j, k, and ℓ.

1 Place an atom in the direction of a line coplanar with two intersecting lines, making equal angles to each. In Fig. 2, $\Phi_1 = \Phi_2$.

The next three options generate two atomic positions (see Fig. 3).

2 Place an atom in two directions making equal angles to the two lines intersecting at the apex. Two positions are symmetrically located on the bisecting plane of the angle formed by the two lines.
In this option, specify the angle Φ and the program generates the positions to have $\Phi = \Phi_1 = \Phi_2 = \Phi_3 = \Phi_4$.

3 Same as above except the angle to be specified is ω

$$\Phi_1 = \Phi_2 = \Phi_3 = \Phi_4$$

4 Same as 2 above, except the program chooses the positions to make all five angles equal. No angle specification is necessary.

$$\Phi_1 = \Phi_2 = \Phi_3 = \Phi_4 = \omega$$

5 Place an atom in the direction of specified bond angle and in the plane having the specified torsional angle.
Note that this option generates the bond from k^{th} atom.
The definition of the sign of torsional angle follows the convention, that is, a positive angle for the clockwise rotation of the plane looking down j - k. (Fig. 4).

6 Place an atom on the direction of a line parallel to the vector $\overrightarrow{jk}$. In Fig. 5, atoms i and j may be the same atom, which is the case in Fig. 5'.

7 Place an atom on the direction of a line parallel to the normal of a plane defined by $\overrightarrow{jk}$ and $\overrightarrow{j\ell}$ in the expression $(\overrightarrow{jk}) \times (\overrightarrow{j\ell})$ (Fig. 6).

10 Calculate the angle between two directed lines formed by atoms i,j and k,ℓ

$\overrightarrow{ij}$, $\overrightarrow{k\ell}$ (distance and angle only)

Cols 8-10 Specify the ith atom. The atom i is the apex of the angle and the starting position of the new bond except inthe option 5.

13-15 Specify the jth atom

18-20 Specify the kth atom

23-25 Specify the ℓth atom. This is used only in the option 0.

26-35 Desired distance from the apex atom i to the generated position(s) in Å units. For option 5 (torsion angle), the distance is from k.

36-45 Angle to be formed between the generated bond and one of the given bond.
This is required in options 2, 3 and 5.

46-55 Torsional angle with a sign for option 5.

60-65 If some identification is required on the generated coordinate card(s), up to six alphanumeric characters may be punched here. They will be reproduced on the output cards.
The field may be left blank.

All generated atomic positions are stored in sequence following the original atoms read in. Therefore any newly generated position may be used as the basis of further generation. As many specifications as necessary may be used until the generated positions fill up the assigned dimension of the atomic array (currently 150).

Output

a) Printer

The following information will be printed:

1) Option 0

Distances: $\overline{ij}$, $\overline{ik}$, $\overline{i\ell}$

Angles: $\angle jik$, $\angle ki\ell$, $\angle \ell ij$, $\angle jip$, $\angle kip$, $\angle \ell ip$

Fractional coordinate for atom p.

2) Option 1

Distances: $\overline{ij}$, $\overline{ik}$, $\overline{ip}$

Angles: $\angle jik$, $\angle jip$, $\angle kip$

Fractional coordinate for atom p.

3) Options 2, 3 and 4

Distances: $\overline{ij}$, $\overline{ik}$ Angle: $\angle jik$

Distance: ip Angles: $\angle jip$, $\angle kip$

Fractional coordinate for atom p.

Distance: $\overline{iq}$ Angles: $\angle jiq$, $\angle kiq$

Fractional coordinate for atom q.

Angle: $\angle piq$

4) Option 5

Distances: $\overline{ij}$, $\overline{jk}$, $\overline{kp}$ Angles: $\angle ijk$, $\angle jkp$ Torsion angle ijkp

Fractional coordinate for atom p.

5) Option 6

Distances: $\overline{jk}$, $\overline{ip}$

Fractional coordinate for atom p.

6) Option 7

Distances: $\overline{jk}$, $\overline{j\ell}$, $\overline{ip}$

Fractional coordinate for atom p.

7) Option 10

Distances: $\overline{ij}$, $\overline{k\ell}$ Angle: $\overrightarrow{ij}\cdot\overrightarrow{k\ell}$

b) Card Output

For each atomic position generated, a card will be punched in the standard coordinate card format of the Structure Factor, Least-squares programs.

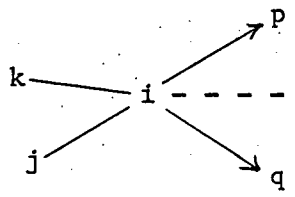
FØRMAT(A4,A2,21X,3F9.6)

Cols. 1-6	Any alphanumeric characters punched on columns 60-65 of the Specification Card will be copied here.	
28-36	x	fractional coordinate
37-45	y	
46-54	z	

<u>Note for Options 2, 3, and 4:</u>

When the program generates two atomic positions with one of those options, the atoms are generated in the following order in terms of the torsional angle.

First atom p: Torsion angle j-i-k-p (+)
j-k-i-p (-)



Second atom q: Torsion angle j-i-k-q (-)
j-k-i-q (+)

Assembly of Cards

Title Card
Unit Cell Constant Card
Control Card
Specification Cards (as many as necessary)

Composition of the Program

1) Main Program

2) Subroutines

AGCØS, CØSAG, DIFV, MATV, MV, NRDIR, VV

HERM - November, 1975
Author: J. Hermans

Brookhaven Crystallographic Computer Program

```
PRØGRAM HERM(INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE7,TAPE8)
```

MODEL BUILDING AND ENERGY MINIMIZATION OF PROTEINS

Manual for using the system

REFINE2

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JUNE 1975

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References

1. J. Hermans and J. E. McQueen, Computer manipulation of (macro)molecules with the method of local change, Acta Cryst. Vol. A, 30, 730-739 (1974).

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3. L. Katz and C. Levinthal, Interactive computer graphics and representation of complex biological structures, Ann. Rev. Biophys. Bioeng. 1, 465-504 (1972).

4. D. Poland and H. A. Scheraga, Energy parameters in polypeptides. I. Charge distributions and the hydrogen bond, Biochemistry 6, 3791-3800 (1967).

5. J. Hermans, D. R. Ferro, J. E. McQueen and S. C. Wei, Use of energy calculations to refine and understand structure and function of proteins, Symposium on Environmental Effects on Structure and Properties, Jerusalem, April 1975, to be published.

Part 1: MODEL BUILDING

1.1. Principle of the program. This program changes a given set of coordinates of a protein to obtain an approximately idealized structure. To do this, the program calculates the following function for each atom:

$$F_{ltr} = \frac{1}{2} \Sigma \left[(\ell-\ell_o)^2 + (\theta-\theta_o)^2 + (\rho-\rho_o)^2\right]$$

Where ℓ is a bondlength, θ a bondangle and ρ a dihedral angle. The subscripts $_o$ indicate the ideal values, and the sum is taken over those fixed parameters which are affected by the position of the atom being considered. Only those parameters are used which belong to a set necessary and sufficient to define the structure. For example, the position of CA of a VAL affects the following parameters:

distance	to N, C and CB
angles	C-N-CA, N-CA-CB, N-CA-C, CA-CB-CG1, CA-CB-CG2, CA-C-N, CA-C-O
dihedrals	CA-C-N-CA, CA-C(-N,-O), N-CA (-CB,-C), CA-CB-(-CG1, -CG2), CA-C-N-CA

The dihedrals N-CA-C-N, C-N-CA-C and N-CA-CB-CG1 do belong in the necessary and sufficient set, but are not fixed, and are therefore not considered, and e.g. the bondangle CB-CA-C is not a part of our minimally sufficient set. In addition to the function F_{ltr}, the program calculates the function F_t

$$F_t = \frac{1}{2} \Sigma (X-X_o)^2$$

Where X is the position of the atom, X_o a target position (here the given starting coordinates). The program attempts to minimize the function

$$G = w_t \cdot F_t + w_{ltr} \cdot F_{ltr}$$

To this end, the first and second derivatives of G ($\underline{G}_1$ and $\underline{G}_2$) with respect to the x,y,z components of the coordinates of the atom are calculated, and the coordinates then changed by $\underline{\Delta}$, so that, in matrix form,

$$\underline{G}_2 \times \underline{\Delta} = -\underline{G}_1$$

i.e., to approximate a new position where $\underline{G}_1 = 0$. This is done for each atom, and the process is repeated more than once for all the atoms. After running through all atoms, the ratio W_t/W_{ltr} should be changed, in order to get a fairly smooth transition from one structure to another.

1.2. Molecular description: tree list and dictionary. In order to find those bondlengths, angles and dihedrals which are involved for any given atom, the program needs for each atom a list of items, called the treelist matrix (cf. Hermans and Ferro, reference 2). The items are, in order, backchain, one forward chain, key for dihedral k_p, key for dictionary k_d; k_p is zero or negative if the dihedral is frozen; if positive, its value is used as a pointer when doing energy minimization. k_d points to a table of ideal values.

The ordering of the atoms and the chaining scheme are subject to requirements approximately as suggested in reference 1. Only a single forward chain is given and for that reason the connectedness of hydrogen atoms is usually not known via the forward chain with the heavier atom to which they are bonded but only via their own backchain. The ordering must satisfy the following requirements. (1) Every atom must be backchained to an atom occuring earlier in the list. (2) For any atom, the forward chain listed in the tree list must be the atom of highest number bonded to the atom. This atom is then also the fourth atom for defining the dihedral for the preceding bond, cf. Figure 2, case I. (3) A hydrogen atom is not given as the forward chain unless hydrogens are the only atoms attacked. With rule 2, this must then be the last listed of the attached hydrogens.

The first atom of the list carries a backchain of zero or smaller, which indicates the 'root'. If the list covers more than one molecule (e.g. Ribonuclease-S), each piece starts with an atom with backchain less than 1. It is unfortunately necessary that all starting atoms have a true degree of exactly 1 (or 0 if this is an isolated atom, e.g. a water molecule without hydrogens). I.e. only a single atom may be backchained to any starting atom.

The dictionary and the tree are created by subroutine TREBIL, on the basis of an input dictionary (TREBIL can drop the hydrogens from the standard input dictionary). The dictionary is usually a member of a partitioned data set. Notice how the dictionary is divided in residues. Extra residues in exactly this form may be given in the same input stream as the sequence (useful if input dictionary and sequence are not in the same stream).

Connection between residues is obtained by specifying (exactly) one backchain smaller than 1 and (exactly) one forward chain larger than the # of atoms in the residue. The exact value of these unsatisfied chains is immaterial. The chains as given in the dictionary are calculated w.r.t. the first atom of the residue.

Bondangles and dihedrals must be in degrees. The cis conformation is given by a dihedral of zero. Bondangles must be $0<\theta<180$. (Consult the current protein dictionary for guidance in building additional entries, or a dictionary for other types of macromolecules.)

Each ideal value is listed with the highest numbered of the atoms which determines it. I.e. bondlength holds for atom and its backchain, bondangle for atom, backchain and double backchain. Dihedral for atom and three backchains. Notice that the indication of a variable dihedral (k_p) occurs at the higher numbered atom of the two on either side of the bond, i.e not with the atom where the value would be listed if the dihedral were fixed.

Table I. Use of the Treelist Matrix

TREE(1) = See section 2.9.

TREE(2) = backchain. Must be less than atom #. Value of zero or lower indicates the start of a new chain.

TREE(3) = highest forward chain. No atom with higher number is backchained to this atom. Value of zero indicates that no atoms are backchained to this atom.

TREE(4) = movability. +1 = movable, 0 = not movable. By subtracting 10 from these two values we indicate slaves of movable or nonmovable atoms (-9 or -10).

TREE(5) = key for dihedral. Value of 0 indicates that the dihedral is frozen. Positive value is a pointer to array VRO containing barrier , multiplicity and origin.

TREE(6) = key to dictionary of ideal values, atomname (and force constants in version 3).

The rules of the preceding par. do not cover one case, namely the definition and use of the dihedral angle at a fork, cf. Figure 1, case II. As said, the dictionary value of ρ for the atom (*) in case I is used to obtain the correct dihedral for the bond (2-b) if this bond is not freely twistable. If it is twistable, as indicated by a positive k_p for atom (b), then the value of ρ is unimportant, except that it may be used to calculate starting coordinates for atom (*) if these had not been provided. Atom(*) is the highest forward chain of atom (b) and is listed as such with atom (b). Any other forward chain of atom (b), such as (+) is found by virtue of its being backchained to atom (b). The value of the dihedral listed with atom (+) indicates by how much atom (+) is out of the plane (1,b,*) by rotation about bond (1-b).

It is an advantage of the use of dihedrals of type II that differences of bondedness, such as between an L- and D-residue are handled effectively, whereas no distinction is made between enantiomorphs when no use is made of type II dihedrals and all the bondangles are idealized, although by doing this one may still obtain a precise conformation. It is an annoying consequence of this very advantage that it becomes essential that names and coordinates of atoms CG1 and CG2 in valine correspond. In many sets of protein coordinates there is no systematic correspondence of this kind.

An L- and a D-residue differ only in a single dictionary element. Simultaneous use of D- and L-residues of the same chemistry requires two entire building blocks in the input dictionary, but only one new atom would be created in the used dictionary (DICT2). However, with use of the CHANge option (cf. 3.5.f) the need for additional entire building blocks can be avoided.

1.3. Ring structures. Ring structures in general must, and, if one so wishes, flat ones may be treated by using the correct chains everywhere. Because of the rules governing forward and backchains, the conformation of the ring near the closure will not be ideally maintained, since the closing connection is not known to most parts of the program. One obtains ring closure by having several additional, dummy or slave atoms, which have the coordinates of real atoms on one side of the closing connection, but are logically connected to the atoms on the other side of the closing connection.

The dictionary of December 1974 distributed with the program uses only a single dummy atom to define a closing bond for each ring, and the bond is known only to one of the atoms on each side of the closing bond. For precise work, at least three dummy atoms must be given on each side of the bond. For example, for proline, one may use the building block of Figure 2a and b. This structure also has the merit of providing flexibility to the ring, by virtue of the nonzero values of k_p for the side-chain. A less flexible preset ring geometry obtains if these k_p are set to zero, and appropriate fixed dihedrals given in the last column. Extended dictionary entries for proline and phenylalanine are given in Figure 2b and c. A similar entry for tryptophan contains 44 atoms, of which 20 are dummies.

1.4. Pit stop for new users. Try building a tree of your choice with your sequence by specifying STOP on the card read following the sequence (cf. 3.6).

1.5. Input molecular listing. A variety of input formats is acceptable. Identification of atoms is by atomname and residue name or residue number. Also, the coordinates may be scaled (to get Å from fractions) and atom and residue names may be translated if they are not as in the standard dictionary.

Three possible systems:

System a. Two types of cards:

i. residue name, # atoms, code
ii. (several) atom name, coordinates

Residue card is distinguished from the atom cards by a unique code. This format is available as so-called elegant output.

System b. i. coordinates, atom name, residue name (atom-plus-residue)

ii. Coordinates, atom name, blank (atom, only)

(cf. Diamond)

System c. Atom name, residue number, coordinates on all cards

(cf. X-ray system)

1.6. Pit stop for use with a new set of data or new problem. Specify GOON at input 3.6 and LTHR at input 3.13 and you will get tree plus coordinates, also a listing of all bondlengths, angles and dihedrals, and ideal values. This is an important check on the input, for example possible exchange of CG and OG in THR, CG1 and CG2 in ILE and VAL, and punching errors.

1.7. Cycle control. For the sake of efficient program execution, the refinement is divided into blocks of cycles over all the atoms (subroutine CNTRL). Control cards can be used to specify if intermediate output is wanted, and to specify the number of cycles and starting and ending weights for the five types of terms. The weights change exponentially from the starting to the final values. In energy refinement, each call of CNTRL causes the calculation of a table of nonbonded contacts.

1.8. Ring closure, margins and flexible zone. As mentioned, ring closure may be obtained by specification of dummy atoms, which are connected to one part of the molecule, but which are 'slaves' of 'master' atoms in another part of the molecule. A slave always has the same coordinates as the masters, and moves only if its master moves. An atom which is its own master and slave never moves. An atom which is a slave is not included in non-bonded interactions, except when it is its own master-slave.

A single flexible zone of contiguous residues may be selected. The real atoms outside this zone will behave as master-slave atoms within the flexible zone.

1.9. Error messages. Many errors are flagged in a unified manner. These are by and large those errors which the user can correct by changing his input. The format of the messages is:

WARNING
ERROR
{SEVERE ERROR} OF TYPE routine, identification #, item (fixed), item (float),
FATAL ERROR [item(char.)

The same item is printed three times with, respectively, I, E and A format. The severity of the error is from 1 through 4, in agreement with the message. Fatal error (4) will cause immediate termination of execution. With severity 2 or 3, execution continues, but later cancellation may occur in case the error code specified as input 3.3(1) is not 'GOON'.

1.10. Storage requirements. The block data subprogram sets the required dimensions. Linkedit the block data subprogram first, then the other modules in any order. The size of the dimensions always should be equal to the starting values of integers which may be reset down (but not up) by the program if storage exceeded requirement. The automatic preparation of consistent block data subprograms is described in section 4.3.

Integer		Associated arrays
NRES	(# of residues in molecule)	SEQ (2,NRES+1)
NAT	(# of atoms in molecule)	X(3,NAT), X1 (3,NAT), TREE (6,NAT)
NMAS	(# of master atoms)	MASTER (2,NMAS+1)
NSLAV	(# of slave atoms)	SLAVE (2,NSLAV)
NADC	(# of atoms in used dictionary)	DICT2 (4,NADC)
NBB	(# of building blocks)	RESNAME (NBB)

The subroutines must be recompiled if NBB exceeds 30. The standard dictionary provides 22 residues. If NBB > 30, the arrays KEYBB and NATBB, of length NBB+1 and NBB must be changed in subroutine TREBIL. The storage for the dictionary is later used for the coordinates. If the number of atoms in the dictionary, NAD>(6*NAT-62)/5 , then one must give the array X (but not X1 or TREE) larger dimensions of (3,(5*NAD+62)/6), and initialize NAD accordingly. Otherwise, NAD must be initialized to zero. (For CDC replace 6 by 3 in the above expressions)

Entries in the dictionary with the same atomname, bondlength, angle and dihedral are combined. The used dictionary (DICT2) is therefore shorter than the input dictionary. The hydrogen atoms may be removed from the dictionary by specifying NOHY under input 3.2.i.

If the above listed arrays are given, the item MODE may be initialized /4HMODL/. Among these arrays, only X1 is optional. If X1 is omitted, MODE must not be initialized to /4HMODL/ or to /4HBOTH/ and may only be given the value /4HENER/. Other arrays must then be included, cf. Section 2.10.

If either MODL or NOHY is specified, then certain subroutines are never called and need not be loaded. These are:

SETLAT, SETABHB, SETBAR, NAYBOR and RFENER.

Part 2: ADDITIONAL INSTRUCTIONS FOR ENERGY MINIMIZATION

2.1. The calculated function for each atom is

$$F_i = K_\ell \sum_j \tfrac{1}{2}(\ell_j-\ell_o)^2 + K_\theta \sum_j \tfrac{1}{2}(\theta_j-\theta_o)^2 + K_\rho \sum \tfrac{1}{2}(\rho_j-\rho_o)^2$$

$$+K_e \sum_j (-A_{ij}/r_{ij}^6 + B_{ij}/r_{ij}^{12} + C_{ij}/r_{ij}) + K_d \sum_j \tfrac{1}{2}E_b\{1-\cos n(\phi_j-\phi_o)\}$$

These are the energy contributions for deformation of (a) bondlengths, (b) bondangles, (c) fixed dihedrals, (d) nonbonded energy and (e) torsional potential. The first 3 terms are also used when model building, the last two only when energy minimizing. (The calculation of the 4th term is done in a new subroutine RFENER, that of the last is done by an extension of the subroutine RFIDEAL used also to calculate the first 3 terms.) Each group of terms is weighted according to the weights K_ℓ through K_d. At the end of the refinement, these should be given values to make F_i the energy of the interactions of the atom i with its surroundings. In this version of the program, all bondangles as a group therefore have the same force constant, as do the bondlengths and the fixed dihedrals.

If the coefficients A, B, C and E_b have been given values to let the unweighted 4th and 5th terms come out in kcal/mole, then we suggest values of the weights of (300, 30, 15, 1 and 1). However, as with the model building it is advantageous to let the weights have different ratios at earlier stages of the refinement. Thus if one starts from a conformation which has been model-built, then one should give terms 4 and 5 relatively high weights in the beginning, and let these come down gradually. And it will be advantageous to let the weight for the bondlength deformation (term 1) be relatively small at some stage.

The program still works with a minimum set of geometric constraints, the same set used by the model building program. One advantage of this is that one program and one dictionary can be used for both purposes. A disadvantage is that if noticeable (usually local) strain in bondangles and dihedrals occurs, then this strain will not be distributed correctly. We have developed another version of REFINE with which the local strain is distributed more correctly over the structure, and which allows the use of a different force constant for each different type of bondlength, bond-angle and fixed dihedral. Any journal articles in which we report results of energy minimization will describe results obtained with that program.

2.2. <u>Intrinsic barriers</u>. These are calculated according to

$$E = \tfrac{1}{2}E_b\{1-\cos n\ (\phi-\phi_o)\}$$

E_b is the barrier to rotation; n the number of minima of the potential and ϕ_o a position of minimum (= zero) energy. The values of E_b, n and ϕ_o are read in routine SETBAR, together with a key, which will be the index of this vector in the array BARR. The key, k_ϕ, used to retrieve the items in the course of the calculation is the fifth item of the treelist matrix, which is set equal to the sixth item in the input dictionary. Zero value of k_ϕ indicates that there is no term to be considered. Each barrier is

taken into account only for any four atoms in the following set: atom i, its backchain, its double backchain, and its main forward chain, which is always the last of the forward chains given in the tree list matrix. The pertinent k_ϕ is listed with atom i, and the twistable bond is, of course, the bond between i and its backchain.

2.3. Non bonded energy. The first two dictionary values are the square roots of A_{ii} and B_{ii}: A_{ii} and B_{ii} are in kcal/mole•A^6 and kcal/mole•A^{12}. The third is the partial charge. These three parameters are read by subroutine TREBIL into array VDW, which is parallel to the array DICT2 which contains atom name and the three ideal geometric parameters. A_{ij} is obtained as $\sqrt{A_{ii}}\cdot\sqrt{A_{jj}}$, etc. The charges, C, are to be given as fractions of the charge of the proton. The 'dielectric constant', DC, initialized in the block data subprogram converts C_iC_j/r with the C's in these units and r in Å, to kcal/mole.

2.4. Neighbor table. The neighbor table is calculated in subroutine NAYBOR. This calculation is made efficient by using Katz & Levinthal's method of 'cubing' (cf. Section 2.8). Three additional common blocks are required. Two of these are workspace used only in NAYBOR (BXVC and IBLKAD). TABLE contains the list of neighbors; if the list is very long, it is written onto a disk file. In that case the block TABLE is used to contain a part of the list. Since new contents of TABLE will be read a number of times during each cycle over the atoms, its length should be chosen for economical input from disk. A value of 6515 × 2 bytes is currently just right for one track. For a small molecule, the length could be decreased, and for a molecule which is just a little too big, the length should be increased, since no disk in- or output is done if block TABLE is never filled.*

The entries in TABLE have the following format. For each atom: a positive integer is the number of a nonbonded neighbor of that atom. A negative number is to be converted to its absolute value, and signifies a hydrogen bonded neighbor. The positive number following a negative entry is a key to retrieve from a separate array the constants A_{ij} and B_{ij} to be used. An entry equal to the number of the current central atom signifies the end of the nonbonded neighbors for this atom. A zero entry is an error.

Atoms further removed than a certain distance are not considered to be nonbonded neighbors. The cutoff distance is the square root of the item RL2, set in the block data subprogram.

2.5. Hydrogen bonds. We use the method of Poland & Scheraga (reference 4) which assigns different A_{ij} and B_{ij} to hydrogen bonded atoms. We use two new arrays: ABHB, containing these A's and B's, and KEYH, a key indicating what H-bonding, if any, is possible, for each atom type. I.e. KEYH is also

* On a machine with 'extended' core the entire neighbor table might be in that part of the core storage, even when the molecule is large.

parallel to DICT2. These arrays are set in subroutine SETABHB. The key is positive for a hydrogen and negative for an acceptor atom, zero for non hydrogen bonding atoms. The two keys are combined as follows to obtain the index to retrieve A and B from the array ABHB:

$$\text{index} = -\text{keyh}_{acc} + n_{acc} \cdot (\text{keyh}_{don} - 1)$$

where n_{acc} is the total number of acceptor types.

A hydrogen bond is considered to be present if, in addition to the types being donor and acceptor, the distance between the donor and acceptor is less than the square root of the value specified by RL2HO, and if the cosine of the angle made by the bonds leading to the two atoms is greater than the value specified for COSMX. This test on the angle made by the bonds does not distinguish between carbonyl and OH oxygens, although it probably should. The test is omitted if either of the bonds is undefined.

2.6. Non bonded cutoff. Since we work with a table of neighbors, there is no problem of a non bonded cutoff creating discontinuities during the calculation. Of course, there may be a small discontinuity when the table is recreated, but we do not believe that this is a serious problem.

However, a cutoff on distance alone is not satisfactory, because one now often excludes a portion of a dipole from the neighbors. The effect of this can be quite severe. One must take care to have the neighbor table represent an electrically neutral environment for each atom (although this may not be possible if there are charged groups in the molecule and counterions in the solvent).

We also require reciprocity of interaction; for example, a bond or a non bonded contact between atoms i and j is to be taken into account at both atoms i and j.

A result of the two requirements is a more complex calculation of the neighbor table. In our current version, electrically neutral groups of bonded atoms are permanently identified. If any atom in one group (I) interacts with any atom of another similar group (J), then all the atoms of group J are included in the list of neighbors of any atom belonging to group I, and vice versa.

2.7. Group table. In each dictionary building block, the atoms are appointed to neutral groups (i.e. groups for which $\Sigma C_i = 0$).

a. Actual groups should have any positive number at the first atom of the group in the listing.

b. A negative number indicates that this atom is not part of a group, and this should be used for any neutral atom.

c. Zero indicates that this atom should be given the same group number as the atom to which it is backchained. Notice again: any time a positive group number occurs, a new group is created. The first atom of a

residue (and any number of atoms backchained to it) may be made part of a group started in the preceding residue, by giving zero for the group number of this (these) atom(s).

A table of groups is created by TREBIL, and a complementary table of atomnumbers ordered by groups (and an associated vector of keys) is also set up (array GRP in block TABLE). These arrays are used only in subroutine NAYBOR.

2.8. Cubing. This is done exactly as described by Katz & Levinthal (reference 3). We use cubes with an edge of 2 Å, giving 3 boxes on the cutoff distance of 6 Å used by us (cf. items NBRAD and RL2 set in block data subrpogram). The number of boxes required is, of course, a function of the size and shape of the molecule. The program will halt with a message if more boxes were required than space had been given for.

2.9. Crystal lattice. If this is asked, the program will generate symmetry related surroundings of the central molecule. The atoms within a 4 Å distance of the (moving portion of the) central molecule will be selected and placed in a pseudo residue named LATT at the end of the molecular listing. Every time a central atom moves, its symmetry related copies will move also; this is not unlike the behavior of slave atoms. The surrounding atoms are not bonded to other atoms (backchain is zero for all of them), and can only participate in nonbonded interactions.

When generating the lattice, one must specify for a number of symmetry related molecules the symmetry matrix and the translation. The new coordinates $\underset{\sim}{x}'$ are obtained from the matrix $\underset{\sim}{M}$, the old coordinates $\underset{\sim}{x}$ and the translation $\underset{\sim}{t}$, with

$$x'_j = \sum_{i=1}^{3} M_{ij} x_i + t_j$$

(The matrix is read in as M_{11}, M_{21}, M_{31}, M_{12}, ..., M_{33}.)

The calculation of the first and second derivatives of the nonbonded energy with respect to the coordinates of any atom is different when the two atoms are a symmetry related pair, unless the symmetry operation is the identity matrix, i.e. this particular copy was obtained as a result of a simple shift of the central molecule. (Because we use a cutoff distance, screw axes in large unit cells do not lead to such pairs.)

This feature makes use of the first column of the tree list matrix, which contains a pointer to the next symmetry related atom. (Zero indicates there are no (further) symmetry related atoms.) For the surrounding atoms, the columns in the treelist have the following meaning:

(1) pointer to next higher atom with same master
(2) backchain (= Ø)
(3) index of the surrounding molecule to which this atom belongs
(4) movability (= 1)
(5) number of the master atom
(6) key to dictionary

These atoms also belong to groups, and the array GRP must be made large accordingly.

2.10 Storage. (cf. Sections 1.10 and 4.3) The following additional blocks are required if the nonbonded energy is to be calculated. Both the 'variable' dimensions and the initial values of corresponding integers are set in the block data subprogram.

block	array
/TABLE/	AREA1 (LREC) halfword
/BXVC/	BXVC (NAT) halfword
/IBLKAD/	KEYBOX (NBX+2) halfword
/ECON/	EPARM (3,NADC) fullword
/HBOND/	ABHB (2,25) fullword, KEYH (NADC) halfword
/GROUP/	GRP (2,NATGR) halfword

Some of the items were defined in Section 1.10. LREC may be chosen equal to (one half) the track size on disk if the neighbor table is to be written on that medium. NBX = number of cubes; NATGR = (number of atoms in groups + number of groups + 2) or (number of atoms) whichever of the two is greater.

If a larger array ABHB is needed, then subroutines NAYBOR, SETABHB and RFENER must be recompiled.

The size of the array /VRO/ BARR (3,20) is determined when compiling subroutine SETBAR.

The dimensions of array /XZ/ X1 (3,NAT) can be given as (3,1) when doing energy minimizations. In that case, MODE must be initialized to /4HENER/; notice the initialization of X1 (3,1). If all the arrays of 1.10 and 2.10 are given, MODE may be initialized to /4HBOTH/. With use of data specification of BOTH or MODL, and if ENER is not specified as the objective, the array X1 will be used to retain the original coordinates, and these will be printed next to the calculated coordinates if one specifies either TREE or LTHR at 3.16.a, or LTHR at 3.17. Therefore, if one wishes this listing (and the differences) when doing energy minimizations, then one uses BOTH as objective and keeps WT(1), cf. 3.16.b, at 0.

In case a crystal lattice is to be generated, one also needs to set NLAX, the maximum number of surrounding molecules, and to allocate the array MTYP in /WTSC/:

/WTSC/	MTYP (NLAX) fullword

Part 3: SEQUENTIAL LISTING OF INPUT DATA AND OPTIONS

The cardreader is assumed to be file number 5, the printer file number 6. It is impossible to work without allocating datasets to files 5 and 6. File 5 is called Input in this section.

3.1. (file: Input) one card; Format (7I5)

6 file numbers, test flag

The file numbers are for	default is	suggested medium
(1) dictionary in	: 7	(cards), (disk - member of p.d.s.)
(2) tree out	: 6	(printer)
(3) coords. in	: 8	(cards), (disk - member of p.d.s.)
(4) coords. out	: 2	(cards), (disk - member of p.d.s.)
(5) sequence in	: 5	(cards)
(6) neighbor table	: 0	must be: disk- sequential data set

(Suggested units in parentheses.) Defaults indicated apply when unit is read as 0. The test flag is best left at zero. If used, it will give a report on the bonds, bondangles etc. taken into account for every atom.

3.2.a.(file: Input) one card; Format (2(A4,6X))

objective, environment

Objective may be one of four choices:

MODL (model building with hydrogens)
NOHY (model building without hydrogens)
BOTH (choice deferred until cycle control specified, Section 3.16)
ENER (energy calculation)

The selected objective is compared with the value of MODE set in the block data subprogram. MODL and NOHY are compatible with data specifications of MODL and BOTH. The objective ENER is compatible with data specification of BOTH and ENER, and the objective BOTH only with a prior specification of BOTH.

Environment may be:

LATT -to specify extension to a crystal structure with use of symmetry operations specified later. (Use this only with energy calculations.)

Other -only the central molecule(s) will be considered.

b.(Input) one card; Format (20 A4)

A title describing this run (80 characters)

3.3 (file: Input) one card; Format 3(A4,6X)

error code, two print codes.

(1) error code:

GOON - refinement regardless of error

blank - no refinement if severe error occurs

other - no refinement in case of error.

These errors do not include the Fortran errors, but only those errors which are flagged by REFINE2 in processing input data.

(2) first print code:

other: entire dictionary will be printed.

GEOM: only the geometric part of the dictionary will be printed.

blank: no part of the dictionary will be printed.

(3) second print code:

blank: large errors in bondlength, etc. will be flagged during execution.

other: this flagging will not occur.

3.4.a.(file: Input) all cards: Format (A4)

i. SELE
{EXCL }
other

ii. residue names (any # of cards only if SELE or EXCL on preceding card)

iii. END

With SELE, only the following residues will be selected from the dictionary. With EXCL, then the following residues will be excluded from the dictionary. With any other specification, the 'name' cards and END must be omitted.

Notice that the description of a residue can be replaced by first excluding it, then reading it in differently (but with the same name) in the supplementary dictionary given ahead of the sequence (Section 3.5).

(The names to be selected or excluded are placed at the end of the array used also for the names of the residues copied from the dictionary. As a result: If more than one half the residues in the dictionary are to be used, then use EXCL, not SELE.)

b.(file: tree in) dictionary (cf. 1,2). Many cards; terminate with END . The first card of the dictionary is a title card which is copied to the printer. The formats are described in Section 3.5.

3.5. (file: sequence in)

Optional: First card may be

(a) i. DICT Format (A4)

Following this card, additional dictionary members may be read, with any number of the following groups of cards:

ii. residue card: A4,6X,I5 (residue name and # of atoms)

iii. atom cards (one or more): A4 (atom name), 5I2 (degree through k_p), 3F5 (bondlength, angle, dihedral), 3F6,22X,I3 (three energy parameters and group flag)

Of the five parameters following the name, only the second (backchain), the third (forward chain) and the fifth (key for dihedral) are used. (The fourth replaces the third when it is the larger of the two.) The last four parameters are only required when energy minimization is to be performed.

iv. END terminates the reading of the supplementary dictionary.

Optional:

(b) i. PIEC (Format A4; must be first card or first card after supplementary dictionary.)

ii. residue #, atom # (Format 2I10, one card, only if preceding card was PIEC card.)

The provided residue and atom # will be used on input and output as the numbers of the first residue and first atom in the molecule, even though internally these numbers are both = 1. (Notice that residue- and atom-numbers in error messages are internal numbers.)

Cards or groups of cards described under c, d, e, f and g may be mixed to produce the molecular description.

(c) residue name Format (A4)

This should be one of the names read as a residue into the dictionary, either under 3.4 or under 3.5.a. Each card will lengthen the molecule by so many atoms.

(d) i. INSE Format (A4)

With this instruction one adds the atoms specified by the next sequence name to the preceding residue, i.e., one increases the atom count, but not the residue count. On the card following INSERT, one specifies the residue and the connectors. Residues to be inserted must have either one or two unsatisfied chains if the insert is to be hooked up to the rest of the molecule. These will be set by the program following the specification of connectors:

ii. Sequence name,KON1,KON2,KON3, KLAS,LEADER Format (A4,6X,6I5)

Inserts can be of three types, depending on the connectivity; see Figure 4. The connectors are: KON1 in x, to y; KON2 in y, to x; KON3 in x or y, to z. Therefore, the identification

of	free floating	is by	KON1 = any,	KON2 = 0 ,	KON3 <= 0
of	side group insert	by	KON1 <= 0 ,	KON2 > 0 ,	KON3 <= 0
of	main chain insert	by	KON1 <= 0 ,	KON2 > 0 ,	KON3 > 0

As is usual in other situations, the values of KON are determined with respect to the current location, the last atom of unit x being counted as 0, the one before that as -1, the first atom of the insert as +1, etc. (This is the case even when the insert actually appears inside the portion already built.) Only the side chain insert may require a value for KLAS If KLAS is nonzero, then the bond before KON1 will become a variable dihedral angle and the class of the new dihedral will be set to the value of KLAS.

The dictionary description of the atom which is designated as KON3 must have a forward chain pointing outside the range of its residue. This must not be true of KON1 in a side chain insert. The atoms of mainchain and free inserts appear after the last atom of the current residue. On the other hand, the atoms of a side chain insert will appear immediately after KON1, if KON1 is not a hydrogen atom, and will replace KON1 if KON1 is a hydrogen atom. Let KON1A be KON1 in the former case, the backchain of KON1 in the latter. The highest listed forward chain of KON1A will be the atom designated as KON2 unless KON1A already has a forward chain greater than KON2.

Examples of use of INSERT

(A) Assume the existence of building block

CSX	3(d	b	f_1	f_2	k_p)
SGX	1	-2	2	0	11
CBX	1	1	3	0	10
CAX	0	2	0	0	0

(which is needed to specify overlap between disulfide crosslinks). Then the following three cards in the sequence (assuming we do not use hydrogens)

```
CSS
INSE
CSX          -2  1  -1  11 10
```

will do the following: Make the first forward chain of SG (atom -2) point to atom SGX (atom +1), identify C of CSS (= -1) for backchaining the following residue, and set k_p for SG to a nonzero value of 10.

(B) Add building block

FMET	2							
CF	1	-1	2	0	1	0	0	0.0
OF	1	1	3	0	0	1.24	0	0.0

Then starting the molecule with

```
FMET
INSE
MET      -1    1    7    blank
```

will give as first residue FMET (formylmethionine), the atoms of MET being chained between the two of FMET and the next residue.

(C) Add three short building blocks

```
HZ        1
HN1   1  -1   2   0   0   0        0     0
HX        1
HN2   0   0   0   0   0   1.00   110   120
STRT      3
HN3   0   0   0   0   0   1.00   110  -120
N     0   0   0   0   0   1.00     0     0
CA    0   0   0   0   0   1.47   110     0
```

The charges of N, HN1, HN2, HN3 are not shown, but should be set to model an NH_3+ group. Many of the zero elements are zero because these are not used. Then use the following cards to begin a chain with alanine

```
HZ
INSE
ALA   0   1   9   0   1
INSE
HX   -9   1  -1   0
```

With this beginning we obtain two extra hydrogens; the first residue is called ALA. The 'chemistry' of the first few atoms is then set with the option described under (f) below.

If the value of the last item (LEADER) is not zero, then the name of the current residue will be changed to the name of the inserted part.

It is possible to give one or more residues with no atoms, and use an INSERT to change the name of any residue to the name of one of these dummy residues.

(e) CAST Format (A4)

This card terminates the chain. A new chain may be started, which will not be logically connected to the other chain(s) here. Always terminate the molecule with this card. NOTE: put this card before ENDS card.

(f) i. CHAN Format (A4)

With this option the types of individual atoms in the molecule can be changed. (Type includes description of: bondlength, bondangle, dihedral and atomname, and in the case of energy calculations also the values of the energy parameters and the group index.) These groups of cards must be placed directly after the cards describing the respective residues.

ii. atom name in residue just built, residue name, atom name to replace the former atom with. (any number of cards. Format: 3(A4,6X).)

iii. END Format (A4); ends this group.

Example: this example completes what we began in example (C) above.

```
CHAN

HN      STRT    HN3
N       STRT    N
CA      STRT    CA

END
```

(The group index of HN1 should be = 1, that of N in STRT = 0.)

(g) i. SOLV Format (A4) ~~(not yet implemented)~~

ii. residue name, integer (k) Format (A4,6X,I5)

these two cards are equivalent to the sequence [(c) followed by (e)] repeated k times. (Put a CASToff card before the SOLV card.)

(h) ENDS Format (A4)

Terminates the construction of the molecular listing.

3.6. (file: Input) {GOON / STOP} one card; Format (A4)

This is a pit stop with which the inexperienced user can test his understanding of tree list matrix and how it is put together.

3.7. (file: Input; cf. Section 2.5) (Skipped if MODL specified)

Several times: groups of 2 or more cards.

Group (a): Type group (2 or more cards)

i. First card: TYPE, type #, {DONO / ACCE} Format: (A4,X,I5,10X,A4)

ii. One or more cards: atomname, {residue name / ALL} Format: (A4,16X,A4)

Group (b): Value group (2 cards)

i. First card: VALU, donor type #, acceptor type # Format: (A4,X,2I5)

ii. Second card: A_{ij}, B_{ij} Format: (2F10)

Type numbers establish correspondence between Type groups and Value groups. (Array KEYH will contain + or - the last entered type number, array ABHB, the values of A and B with the indexing scheme described in 2.5.)

Termination (c): Reading of END rather than TYPE or VALU terminates.

Notes: A key can be set using ALL, then reset using a residue name. A key can be set to zero (not a hydrogen bonder). The order in which the groups are presented is immaterial.

3.8. (file: Input; cf. Section 2.2) many cards; last is END
(Skipped when MODL specified)

(a) any number of times:

spec, index, 0.5×barrier, multiplicity, value of χ where E = 0.
(A4,I6,3F10.2)

(b) END (format A4)
(angle in degrees)

3.9. (file: Input) Input preparative to reading coordinates.

(a) # translated atomnames, # translated residue names (Maximum = 10)
(2I4)

(b) atomname in input, atomname in dictionary, residue name in dictionary. several cards; Format 3(A4,6X); as many cards as specified under (a).

(c) residue name in input, residue name in dictionary. several cards; Format 2(A4,6X); as many cards as specified under (a).

(d) scale factors (3F10.5). If first is blank or zero, all three factors are set to unity. Otherwise blank will give factor of zero!

(e) and (f) depend on the type of molecular listing which is used as input.

In all systems, the coordinates are assigned to the atom of the same name in the current residue. The systems differ in the method by which a change in residue number is flagged. The options are:

A. The use of a special card (residue card) identified by a code.

B. The use of a special field, containing the next residue's name or number (blank = no change in residue).

C. The use of a common field containing the residue number, a change being evident from the change in number, (a blank or the same number as before meaning no change).

3.9. (cont'd)

(e) Input: three format specifications, a code and a flag. Format: (20A4)

On one card, three separate format specifications, each enclosed in parentheses. The first 20 columns contain the format for reading the coordinates, columns 21-40 contain the format for reading the residue name or number and the code-field and columns 41-60 that for reading atomname. Notice that sometimes all information is present on the same card; all cards of the molecular listing are read with A-format, and decoded (=reread) up to three times. (One uses X-format to skip e.g. the atomname when re-reading the coordinates from the card image.) Furthermore, the penultimate 4 columns on the format card can contain a code for distinguishing the residue cards = cards not containing atomname and coordinates. These are identified by having this string in the columns specified by the second item of the second format given as input e. However when the last 4 columns are blank, this code is ignored, and information about residues is expected on (some of) the atom cards. (Notice that the code may be = all blanks.)

(f) NAME {XRAY } other Format (A4)

NAME specifies that residue names are used for determining residue boundaries.

XRAY specifies that the input atomnames will be 'split', as in xray system cards, and that residue numbers are used for determining residue boundaries.

Any other spec implies that residue numbers are used for sequencing, without the split atomname option.

(For examples, see Figure 5)

3.10. (file: coordinates in) many cards

molecular listing. This listing contains atomnames, residue identification and coordinates. The input of the molecular listing terminates with the reading of (a) a card having 'ZZ' for atomname, (b) a card belonging to a residue with number higher than is needed for the molecule specified under 3.5 (or with End of file - not yet implemented).

3.11. (file: Input) one card; Format: 2(A4,6X)

{ADDA / NOAD} and a spec

If ADDALL is specified, all atoms whose coordinates were not read in will have coordinates computed, and if, in that case, 'spec' was not blank, then the first 10 cycles of refinement will be devoted to improving the positions of the atoms (model building only) since ADDALL does not always give a perfect result (e.g. when the added atoms bridge a gap).

3.12. (file: Input) one card; Format: (A4)

{SLAV / NOSL}

This section skipped when NOSL specified.

(a) i. AUTO (optional first card) Format (A4)

Not yet implemented modification of 3.9

Input 3.9.f may contain two words (format: 2(A4,6X)). If the first is NAME, then the second word determines the assumed origin of the input listing

ALL: first residue read in is #1
other: this residue has the same number as the residue set with the PIEC card at 3.5.b.

Residues below the range will be skipped. If a residue is encountered above the range, reading terminates with a warning. Out of order residues will be flagged and processed according to the residue number on the data cards. Misnamed residues will be flagged and processed as the next residue in the sequence.

ii. residue names (several cards, up to 10)

iii. END

Each atom with 'X' or 'Y' in its name in a residue of a type read in after AUTO will become the slave of that atom in the same residue with name identical to the portion of the name of the slave preceding the 'X' or 'Y'. E.g. CDX2 will become the slave of CD.

(b) Residue name, residue number, atomname of master, then same three items for slave, Format: 2(A4,X,I5,X5,A4,X)

Termination: ENDM (Format A4)

These items must be left blank for master, if master is same as in preceding card. The masters must be given in increasing order of atom number.

If in any residue any masters are assigned using method b, then the automatic action will not take place. I.e. if any master is assigned explicitly, then all masters in that residue must have all their slaves assigned to them explicitly.

3.13. (file: Input) one card; Format: 3(A4,6X)

{REFI / STOP / TREE / LTHR} , identification, form of output list of coordinates

(i) REFI will give refinement; none of the others will.
LTHR will give no refinement, will give list of bondlengths, angles, dihedrals, and a tree list with coordinates.
STOP will give neither of these listings.
TREE will give only treelist and coordinates.

(ii, iii) Output of coordinates in form which can be reread by this program will occur if form is specified as XRAY or ELEG. The identification will appear on the output records, also at head of list of bondlengths, etc. Specification of ORTE will give cards which can be used to draw plots with ORTEP.

If REFI was specified, the result of the refinement will be saved in the specified form. If the program does not complete normally, nothing will have been written on the file specified for coordinates out.

3.14. (file: Input) one or two cards

i. {LMIT / other} one card; Format: (A4)

ii. two limits. one card, only if preceding card read LMIT; Format: (2I5)

Only if the first card reads LMIT, a card actually containing the limits is to be provided. Only the atoms within the (inclusive) range spanned by the residues specified as limits will move.

3.15. (file: Input. Two or three groups of cards) This input given only if LATT specified at 3.2.a.(2)

a. block for limit on atoms to be copied to lattice (two cards, optional)

i. LMIT (A4)
ii. lower limit, upper limit (2I5)

b. block for symmetry operations

i. type, matrix (5X,I5,9F7)

as many cards of this kind as necessary to a maximum of 6
1 < type < 6. Type values should be different.

ii. END (A4)
terminates this block

Note: If the last 6 values of the matrix are zero, then the first three elements become the diagonal of the matrix.

c. block for molecules to be generated

i. type, translation vector (5X,A5,3F7)

type can be 1 through 6 and should correspond to one of the supplied types.
A maximum of 20 cards can be given.

ii. END (A4)
terminates this block

Action: Each of the specified atoms will be moved to a new position $\underset{\sim}{X}' = \underset{\sim}{M} \times \underset{\sim}{X} + \underset{\sim}{t}$, where $\underset{\sim}{X}$ are the coordinates, $\underset{\sim}{M}$ the matrix of given type and $\underset{\sim}{t}$ the translation. The matrix should be a rotation matrix, the translation is to be given in Angstroms.

Note: If the matrix type of a surrounding molecule is given the value zero, then no rotation is performed, only a translation.

3.16. (file: Input) several times (2 or 3 cards); last card has 'zero'

One or more instructions for the control of the next group of several cycles of refinement.

(a) # of cycles, {PRIN / LTHR / other} Format: (I5,5X,A4)

Zero # of cycles is used in order to cause normal termination of program execution.

Specification of PRIN will cause printout of tree list and coordinates of the movable part, only.
Specification of LTHR will cause printout of bondlengths, bondangles and dihedrals, then of tree list and coordinates.

(b) {OLDW / other}, weights Format: (A4,6X,6F10)

One or two of these instructions must be given. Last one may not have 'OLDW' specified. Specification of 'OLDW' implies that the following weights are the starting weights for the next cycles. Otherwise, these are the final weights. (The weights change exponentially.) Specification of any final weight as zero will cause that weight not to change. The weights are read in this order:

1:	for approach to target	$(X - X_o)^2$
2:	for idealization of bondlengths	$(\ell - \ell_o)^2$
3:	for idealization of bondangle	$(\theta - \theta_o)^2$
4:	for idelaization of dihedrals	$(\rho - \rho_o)^2$
5:	for vanderWaals & repulsive energy	$-A/r^6 + B/r^{12}$
6:	torsional energy	$\frac{1}{2}E_o \{1-\cos n(\rho-\rho_o)\}$

The weights (array WT) are set and reset in subroutine CNTRL. The members of WT are used for different purposes in correspondence with the above scheme.

3.17. (file: Input) one card; Format: 3(A4,6X)

STOP
{TREE}, identification, form of output list, printcode
LTHR

Except for the absence of the option REFI, the resulting action is as for 3.13. The printing of the treelist can be controlled as follows:

blank: only the moving atoms will be listed
other: the entire central molecule will be listed
LATT: list will describe all atoms; i.e. both in molecule and in crystal

Part 4: PROGRAM STRUCTURE, ERROR MESSAGES, BLOCK DATA

4.1. Program structure. Figure 6 shows the relation between large data structures, program elements, input commands and input and output data structures. Program elements used only once are white. Overlay of the colored routines on the core used by the white routines is obviously advantageous. Elements marked in red are used when doing model building calculations, those marked in yellow are used when doing energy calculations. One does not need the disk file in energy calculations with small molecules.

4.2. List of error messages.

Error type	Meaning of error	Severity	Meaning of item
no message	Terminates because of earlier errors		
FIXTREE1	Atom backchained to atom with too low a forward chain	3	atom #
FIXTREE2	Forward chain below atom's number	3	atom #
FIXTREE3	Atom's f.w. chain to atom with backchain not equal to that atom's #	3	atom #
FIXTREE4	Termination because of one of the above errors		
AYBOR1	Too many boxes	4	number of boxes
NAYBOR3	'First' atom in group, but group already begun	4	current atom #
NAYBOR4	More groups under simultaneous consideration than storage permits	4	atom #
READX1	Number of residue not equal to current or one higher	2	residue number
READX2	Name of next residue ≠ name acc. to sequence	2	residue name
READX3	No atom of this name in residue	3	atom name
READX4	Residue number above range of molecule available	1	0
READX5	Double assignment	3	atom number
REFINEB	Specified objective = BOTH, wrong MODE	4	MODE
REFINEE	" " = ENER, " "	4	"
REFINEM	" " = MODL, " "	4	"
REFINEN	" " = NOHY, " "	4	"
FINE1-A	Wrong instruction for setmarg (not SLAV or NOSL)	4	instruction
RFENER1	Zero atom # as neighbor	4	current atom #
SETABH1	Type not 'DONO' or 'ACCE'	2	type
SETABH2	Donor or acceptor # out of range	3	donor #

Error type	Meaning of error (action)	Severity	Meaning of item
SETBAR1	Index below zero or too high (>20)	1	index
SETLAT1	Type of matrix of symmetry not in range 1 thru maximum permitted (= 6)	2	type
SETLAT2	Type of operation not within range 1 thru 6 or this matrix has not been read in	2	type
SETLAT3	More symmetry operations than maximum	2	maximum
SETLAT4	Have generated too many atoms	4	atom #
SETMARG1	Residue name not according to number in sequence on master-slave card. (Use number, ignore name.)	3	residue name
SETMARG2	Atom name not same as any in residue. (Skip this pair.)	3	atom name
SETMARG3	More masters and/or slaves than storage. (Stop)	4	DIMENS
SETMARG4	Residue number is outside range	3	number
SETMARG5	Cannot find master with appropriate name	3	atom #
MARG6	Too many 'automatic' residues	3	residue name
SETMARG7	Automatic residue longer than allowed in setmarg	3	residue #
TREBIL1	Not enough storage in dictionary, treelist or blank common	4	DIME
TREBIL2	Preceding building block does not have an unsatisfied forward chain. (Hookup will be in error.)	3	atom # of atom with unsatisfied backchain
TREBIL3	Residue name not in dictionary	3	name
TREBIL4	Third connector for insert does not have an unsatisfied forward chain. (Will give mistake in tree list.)	3	3rd connector
TREBIL5	Atom with group # = zero	3	atom #
TREBIL6	Too many selected or excluded names	3	name
XOUT	Manner specified for output molecular listing was neither blank, XRAY, ELEG nor ORTE. (Stop)	4	specified manner

The severity accorded to each error is a matter of taste. It is not difficult to modify the severity: Find the appropriate statement CALL ARROW and alter the first parameter. Any particular message can be given at only one place in the program.

4.3. BLOCK DATA Subprogram preparation

This can be done with a Fortran main program. The input to this program consists of cards containing keyword and value.

Format (A4,1X,I5), (A4,6X,F10) or (A4,16X,A4), depending on the data type of the value.

The table gives all keywords their associated types and shows when a value is to be provided.

Table I. Input Specifications for Make-block-data Program

		keyword	integer	real	alphabetic
MODL	ENER	MODE[a]			X
X	X	NRES	X		
X	X	NAT	X		
do not use!		NBB	X		
X	X	NADC	X		
do not use!		KTES	X		
X	X	NMAS	X		
X	X	NSLAV	X		
X	X	NAD	X		
	X	NDON	X		
	X	NACC	X		
do not give		NBRA	X		
	X	NBX	X		
	X	NATG	X		
	opt.	DC[b]		X	
	opt.	RL2[b]			
	X	LREC	X	X	
	X[c]	NLAX	X		
opt.	opt.	JSAV[d]	X		
X	X	END			

a) The allowed values of MODE are: 'MODL', 'ENER' and 'BOTH'.

b) Defaults will prevail if not set.

c) Provide a value for NLAX only in case a crystal lattice is to be generated.

d) JSAV if set to 1 will generate an array for saving one word for each input atom at reading time, to be copied to output mol. listing.

Result. The output of the Make-block-data program is a source listing of the block-data subprogram, and can be compiled as the first loaded portion of the refine program.

Remark. The program uses Tape # 1 for data input (INPUT or SYSIN), tape # 3 for messages (OUTPUT or SYSPRINT) and tape # 6 for the output listing of the subprogram.

4.4. Saving additional input data for later output.

Save a word for each atom in input stream (A-format).

1. Set JSAV to 1 when making blockdata. This will give an array of dimension (NAT) in block THERMO.
2. If the word to be saved for Atom #1 is blank on the card, it will become 'Ø' (left adjusted).
3. Atoms for which no cards were given in the input will have the field set to 'blank' on output.
4. The field will be read according to the fourth item in the format for reading the coordinates (cf. input 3.9.e, columns 1-20.)
5. Output of this field occurs in subroutine XOUT. (Has not yet been implemented.)
6. The storage for block THERMO should ideally be in 'slow' or 'extended' core.

(For users of other than IBM 360)

Part 5: IMPLEMENTATION DEPENDENT FORTRAN STATEMENTS

5.1. Halfword integer arrays have been used where desirable.

5.2. Main program: CALL DATE (IDATE) to obtain calendar date.

5.3. System 360 Fortran does not have comparisons with characterstring constants. As a convention I have in all cases named the variable, which is given the desired constant value in a DATA statement, by concatenating '$' and the 4 characters of the value. E.g. $TREE is initialized to 4HTREE and $ to a blank fullword. (In CDC version 'I' or 'IQ' replaces each '$'.)

I have used three different methods for <u>character manipulation</u>.

5.4. In subroutine XOUT atomnames are to be split. E.g. CG1 into C and G1, but FE3 into FE and 3. The first half of each name is tested versus the names of an array (presently: FE, NA....), and split into one and three if <u>not</u> found there and into two and two if found. The splitting is done using equivalent arrays of bytes and half words, overlapping the fullword containing the name (ANAM).

5.5. In subroutine READXX split atomnames must be put together. C and G1 must become CG1; FE and 3 must become FE3. Arrays of bytes are equivalent to several words. The second character of the first part of the name is tested by moving the second byte of the name into an otherwise blank work, and comparing this with a blank word. The new name is obtained by moving bytes.

The cards containing the coordinates are read with A-format, then reread, which is done with a read from pseudo unit 99. The rereading is done several times.

5.6. In subroutine TREBIL a test is done on all atomnames in the dictionary to see if they begin with H. The test is performed by calculating the logical AND of the name and the hexadecimal mask FF 00 00 00, and comparing the result with the hexadecimal field 80 00 00 00.

5.7. In the CDC version of the program in READXX and XOUT the string handling operations are done with DECODE and ENCODE statements. The meaning of these statements is as follows

DECODE (80,15,FIELD) VAR1, VAR2...

is similar to a READ (n,15) VAR1, VAR2, ... I.e. <u>15</u> stands for a Format number or variable Format name, <u>VAR1, VAR2</u> for a list of variables to be read. Instead of from tape number <u>n</u>, the characterstring to be decoded is taken from the area FIELD. The number of characters in the field to be read (80) is also indicated. ENCODE works the other way round, i.e. produces a character field from variables. If one uses A-format, these statements produce rearrangements and concatenation of strings. For example, a DECODE with format (1X,A1) produces a variable with as first chacter the

second character of the field; the remaining characters of the variable will be blank. Or, ENCODE of two variables with format (A2,A2) will produce a field containing the first two characters of the first variable, then the first two characters of the second variable and the remainder blank. But the field is of course also a variable which can be used in subsequent statements.

In CDC Fortran the statement

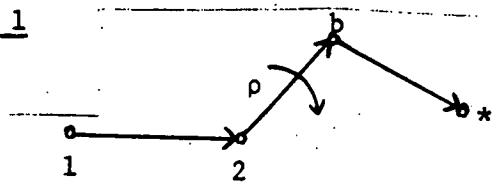
```
VAR = A.AND.B
```

produces in VAR the logical 'and' function of the words A and B. The masking (in TREBIL) is now done with octal fields of 10 characters.

The wordlength is most often assumed to be 4. This works fine with machines having longer wordlength, except when the masks are used. (In the CDC version this has been taken care of.)

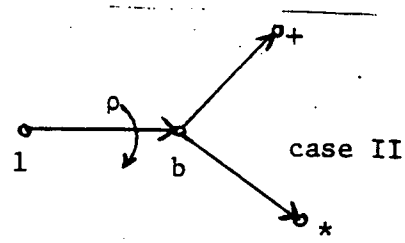
FIGURES

Figure 1



ρ changes distance from 1 to *

case I



case II

ρ changes distance from + to *

In both cases atom '*' is the highest listed forward chain of atom b. In case II + is another atom bonded to b in the forward direction. The forward chain for + need not be listed with atom b. The arrows follow forward chaining.

Figure 2a. Better building block for proline

PRO 13

		d	b	f_1	f_2	k_p	ℓ	θ	ρ
(1)	N	2	-1	2	7	0	1.32	114	0
(2)	CD	1	1	3	0	1	1.47	123	180
(3)	CG	1	2	4	0	3	1.53	109	180
(4)	CBX	1	3	5	0	3	1.53	109	0
(5)	CAX	1	4	6	0	3	1.53	109	0
(6)	NX1	0	5	0	0	0	1.47	109	0
(7)	CA	2	1	8	12	1	1.47	123	180
(8)	CB	1	7	9	0	3	1.53	109	-120
(9)	CGX	1	8	10	0	3	1.53	109	0
(10)	CDX	1	9	11	0	3	1.53	109	0
(11)	NX2	0	10	0	0	0	1.47	109	0
(12)	C	2	7	13	14	2	1.53	110	0
(13)	O	0	12	0	0	0	1.24	121	180

	PRO			24					
1	N	1	-1	13	0	0	1.32	114	0
2	CD	1	1	5	0	1	1.47	123	0
3	HD1	0	2	0	0	0	1.10	110	120
4	HD2	0	2	0	0	0	1.10	110	120
5	CG	1	2	8	0	3	1.53	110	0
6	HG1	0	5	0	0	0	1.10	110	120
7	HG2	0	5	0	0	0	1.10	110	-120
8	CBX	1	5	11	0	3	1.53	110	0
9	HB1X	0	8	0	0	0	1.10	110	-120
10	HB2X	0	8	0	0	0	1.10	110	120
11	CAX	1	8	12	0	3	1.53	110	0
12	NX1	0	11	0	0	0	1.47	110	0
13	CA	1	1	23	0	1	1.47	123	180
14	HA	0	13	0	0	0	1.10	110	120
15	CB	1	13	18	0	3	1.53	110	-120
16	HB1	0	15	0	0	0	1.10	110	120
17	HB2	0	15	0	0	0	1.10	110	-120
18	CGX	1	15	21	0	3	1.53	110	0
19	HG1X	0	18	0	0	0	1.10	110	-120
20	HG2X	0	18	0	0	0	1.10	110	120
21	CDX	1	18	22	0	3	1.53	110	0
22	NX2	0	21	0	0	0	1.47	110	0
23	C	1	13	25	0	2	1.53	110	0
24	O	0	23	0	0	0	1.24	121	180

Figure 2b. Building block for flexible proline with hydrogens, providing complete ring closure.

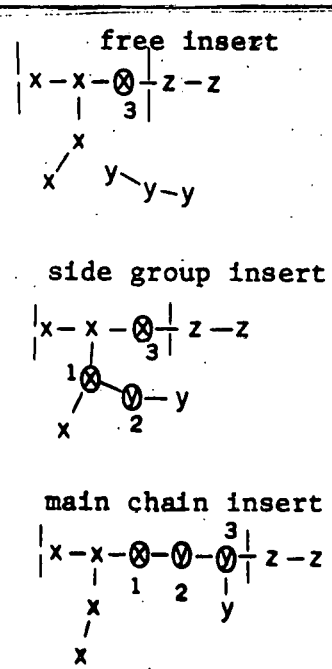


Figure 4. x = residue already there, y = insert, z = next residue. 1, 2 and 3 indicate KON1, 2 and 3. Finally, there will be 2 residues, i and i+1, separated by drawn solid boundaries. Connectors are circled.

	PHE			30					
1	N	1	-1	3	0	0	1.32	114	180
2	HN	0	1	0	0	0	1.10	123	180
3	CA	1	1	31	0	1	1.47	123	180
4	HA	0	3	0	0	0	1.10	110	120
5	CB	1	3	8	0	3	1.53	110	-120
6	HB1	0	5	0	0	0	1.10	110	120
7	HB2	0	5	0	0	0	1.10	110	-120
8	CG	1	5	20	0	5	1.53	110	180
9	CD1	1	8	11	0	0	1.40	120	0
10	HD1	0	9	0	0	0	1.10	120	180
11	CE1	1	9	13	0	0	1.40	120	180
12	HE1	0	11	0	0	0	1.10	120	180
13	CZ	1	11	15	0	0	1.40	120	0
14	HZ	0	13	0	0	0	1.10	120	180
15	CE2X	1	13	17	0	0	1.40	120	0
16	HE2X	0	15	0	0	0	1.10	120	180
17	CE1X	1	15	19	0	0	1.40	120	0
18	HE1X	0	17	0	0	0	1.10	120	180
19	CGX	0	17	0	0	0	1.40	120	0
20	CD2	1	8	22	0	0	1.40	120	180
21	HD2	0	20	0	0	0	1.10	120	180
22	CE2	1	20	24	0	0	1.40	120	180
23	HE2	0	22	0	0	0	1.10	120	180
24	CZX	1	22	26	0	0	1.40	120	0
25	HZX	0	24	0	0	0	1.10	120	180
26	CE1X	1	24	28	0	0	1.40	120	0
27	HE1X	0	26	0	0	0	1.10	120	180
28	CD1X	0	26	0	0	0	1.40	120	0
29	C	1	3	31	0	2	1.53	110	180
30	O	0	29	0	0	0	1.24	121	180

Figure 2c. Building block for phenylalanine, providing complete ring closure.

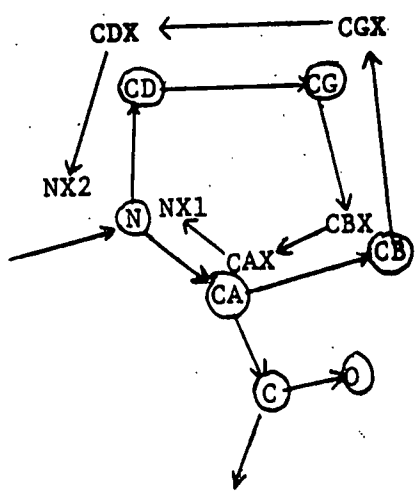


Figure 3. Bonding scheme for the PROX residue with closing connection at CB-CG. Real atoms are circled, the others are 'slaves'. The arrows follow forward chaining.

Figure 5. Examples of input molecular listings and appropriate control cards.

A. The "Elegant" system has residue cards and atom cards. This kind of listing is obtained as output if ELEG is specified under input 3.14 (ii).

```
                1         2         3         4         5         6         7         8     column #
 1    5    0    5    0    5    0    5    0    5    0    5    0    5    0    5    0    5    0
.     5     ALA                              ****                                          . (new residue
.    27  N       5              3.04        4.13        -0.35                              .
     .....
.    29  CB      5              2.19        0.90        -2.03                              .
     ....

.     6     LEU                              ****                                          . (new residue
.    33          6              5.1         7.0         -.07                               .
     etcetera
```

The above listing can be read using two different sets of inputs e and f, namely:

```
e.   (20X,3F12)          (10X,A4,16X,A4)      (7X,A4)                          ****   +.
f.NAME                                                                                    .

     or

e.   (20X,3F12)          (I5,25X,A4)          (7X,A4)                          ****   +.
f.NUMBER                                                                                  .
```

The atomnumbers and residue numbers which occur on the cards are ignored.

B. Xray system type listing.

Sample card:

```
. C 12 G2          12.07     13.98     -2.11                                              .
```

Inputs e and f:

```
e.  (10X,3F10)           (3X,I2)              (X,A2,2X,A4)                                .
f.XRAYSYSTEM                                                                              .
```

C. Molecular listing following Diamond.

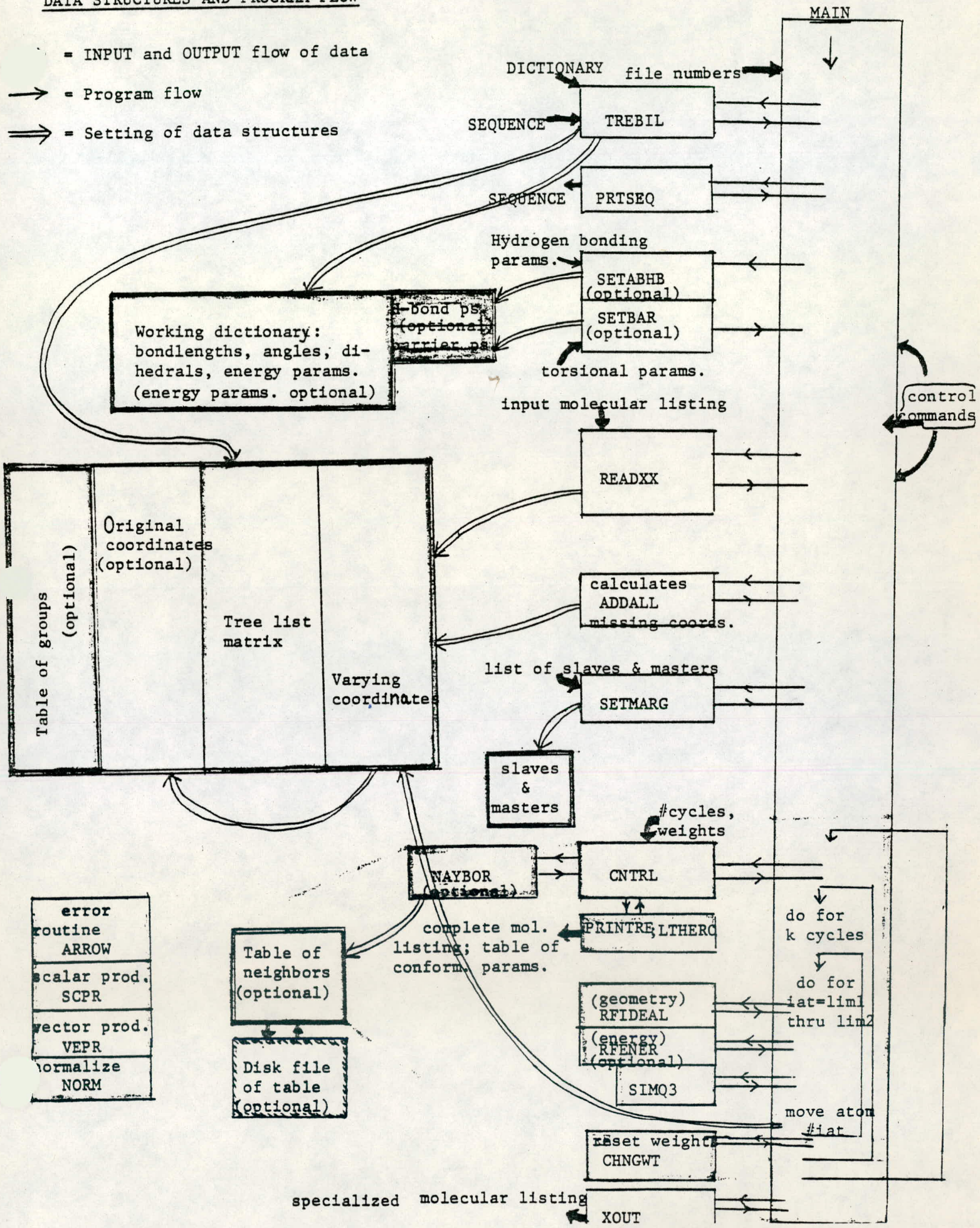
Sample cards:

```
.          5.1       2.0       3.9                                ALA       N            . (new residue)
.          3.5       2.1       4.0                                          CB           .
```

Inputs e and f:

```
e.  (3F10)               (64X,A4)             (72X,A4)
f.NAME
```

Figure 3.
DATA STRUCTURES AND PROGRAM FLOW



(To be inserted in manual)

Part 6: COMPARE facility of the REFINE system

6.1. This allows comparison of two structures, $\underline{X}$ and $\underline{X}_1$. One of the two conformations ($\underline{X}$) is translated and rotated so as to minimize the sum of the squares of the deviations, $F = \sum_i (\underline{X}-\underline{X}_1)_i^2, i=1,2,\ldots,n$ (number of atoms) (Cf. S. C. Nyburg, Acta Cryst. B30, 251, 1974. The method used by us to minimize F is not that described by Nyburg.)

The molecular description (sequence, etc.) is specified as in REFINE. Then two molecular listings are read in. The order and names of atoms as well as the card format may be different in the two listings, but residue numbers must correspond. The listings need not be complete.

After comparing two structures, other pairs of conformations of the same molecule may be compared.

It is possible to indicate what atoms are to be selected to obtain coincidence by rotation and translation, and what atoms are to be totally ignored. Atoms for which no coordinates are given in one set or the other are also ignored. The program uses the first column of the tree list matrix as an index to show the way each atom is to be treated.

6.2. Required modules:

Block data subprogram prepared with specification of MODL or BOTH for MODE
Main for compare
TREBIL
PRTSEQ
READXX
ORIENT
PRINTRE
ARROW
SCPR (a part of MATH)

6.3. Order of comparisons in one job

In principle the same conformation can be used in several comparisons. For example, consider comparisons of three conformations: 1, 2 and 3. First ask for a comparison of 1 and 2, then of 1 and 3. This presents no problem; description 1 is only read in once and is moved into store before reading #3. But if one now asks for comparison of 2 and 3 this will only work if two copies exist of molecular listing 2 or if the single copy can be read and read again. (In either case, the control cards for reading this listing must be repeated in the input stream.)

6.4. Input to the program

1. Three file numbers one card, Format (3I5)
   (1) for reading dictionary
   (2) for reading sequence
   (3) for output of coordinates

2. {MODL / NOHY} one card (A4)

   NOHY causes hydrogens to be dropped from dictionary
3. error code one card (A4)
   Cf. manual 3.3.
4. Input for constructing treelist matrix according to sections 3.4 and 3.5 of the manual.

5. Various control groups. These are processed in order of appearance.

a. Read group

i. READ one card, Format (A4)

ii. Fortran I/O unit number, 20 character title one card (I5,15X,5A4)

This command causes a molecular listing to be read on the specified unit. Notice that every Read group must be followed by the appropriate control cards for reading coordinates, cf. manual, section 3.9. After the listing has been read, the unit is rewound (unless the unit number is 5).

b. Store group

i. STOR one card, Format (A4)

This command causes those coordinates which were read in with the last Read command to be copied into the store array (X1). The old contents of X1 are obliterated.

The contents of coordinates not in storage (X) will be altered by translation and rotation to obtain the optimum fit with respect to the coordinates in storage (X1).

c. Selection group

i. SELE one card, format (A4)

ii. atom name, residue name, index, residue 1, residue 2
one or more cards (2(A4,6X),3I5)

iii. END one card, format (A4) terminates the group

If atom name is blank, then the given index is assigned to all atoms in the specified residue type. If the last three characters of atom name are ***, then the index is set for all atoms (in the specified residue type) of which the names begin with the first character of the specified atom name .

If residue name is blank, then the index is assigned to all atoms of the specified atom type.

The atoms are used in the comparison with weights selected from an array using the assigned index. (The value of index is stored as TREE(1,I), where I is the number of any atom meeting the other criteria on the selection card.) The assigned indices remain in effect for all subsequent comparison, unless explicitly changed by another selection card.

$0 < \text{index} \leq 10$: atoms used in positioning according to weight
index = 0: atoms used in comparison, but not in positioning (unless the index is set specifically, the default is index=0)
index < 0: atoms ignored

These operations are carried out for the type of atoms specified via the names, lying within the range of residues 1 through 2. If residue 1 is zero, they are done for all residues. If residue 1 is not zero, but residue 2 is zero, they are done only for residue 1.

Examples of Selection cards

card 1.	SELE				
card 2.		1			
card 3.	H***	-1			
card 4.	C	2			
card 5.	N	2			
card 6.	CA	2			
card 7.	FE	3	12		
card 8.	END				

Results will be as follows:
card 2: all atoms are given index = 1.
3: all hydrogens are given index = -1, i.e. will be ignored.
4,5,6: all main chain atoms are given index 2.
7: FE in residue 12 is given index 3.

The order of these cards is important. Card 2 would override any earlier assignments.

d. Weight group
i. WEIG one card (A4)
ii. ten weights one card (10F5)

e. Compare group
i. COMP one card (A4)

ii. {PRIN / other}, identification, manner one card, (3(A4,6X))

This causes the comparison to be executed. Specification of PRIN will invoke PRINTRE, i.e. give output of treelist matrix, double set of coordinates, shifts and distances.

manner = blank - no action
= {ELEG / XRAY / ORTE} gives corresponding output of coordinates, cf. manual section 3.13.
= other - error, which causes termination

f. STOP (one card) ends execution

6.5. Procedure for special case

Suppose we want to align a large molecule according to the position of a small subset of this molecule in some other, not necessarily related structure. For instance: align Hipip so that the Fe-S cluster is best coincident with an Fe-S cluster of ferredoxin.

i. Make a 'molecular listing' of the atoms selected from ferredoxin, assigning residue numbers and atom names which are the same as those of the atoms in Hipip which they are to match.
ii. Read this listing with the first READ instruction and follow up with a STOR.
iii. Read the Hipip listing with the second READ instruction.
iv. COMPare.
(Weights and indices have to be set also.)

Brookhaven Crystallographic Computer Program

NAME: INVTRP TIME: $\leq 20_8$ Secs

CORE: 20 K_8

PROGRAM INVTRP(INPUT=200,OUTPUT=400,PUNCH=200,TAPE5=INPUT,TAPE6=OUTPUT, TAPE7=PUNCH)

Purpose

This program will accept cards bearing 3 x 3 symmetry matrices (in row order) invert the matrices and form their transposes. The transposed inverted matrices together with their number then form the substance of an output file which is a card deck image constituting a BLOCK DATA subprogram. The subprogram is named SYMOPS, its function is to preset the contents of the named COMMON/SYMEQV/ in the program AVSORT.

Background

In order to average symmetry equivalent reflections some means must be provided to inform the sorting and averaging program how to transform the indices supplied into those appropriate to the unique portion of reciprocal space selected by the user. For orthorhombic or lower diffraction symmetries this is trivially easy but to do so while retaining both flexibility and generality in a high symmetry group can become exceedingly complex. This program both generates and aids in the supply of the reciprocal space symmetry information; for further details of its usefulness the reader is referred to the AVSORT write-up.

Symmetry equivalent positions in real-space can be considered to be related by a symmetry matrix and a translation vector eg. if we say x', y', z' = 1/2+x, 1/2-y, -z then:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \underset{\sim}{M} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \vec{t}$$

where $\underset{\sim}{M} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ and $\vec{t} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$

both $\underset{\sim}{M}$ & $\vec{t}$ together constitute a real-space symmetry operator.

We can therefore represent the symmetry of real-space with a set of operators such as the above. The diffraction pattern (reciprocal space) has its own symmetry which depends upon that of the real space in combination with the symmetry of the diffraction process. This means that:

(i) Except in special circumstances all diffraction patterns are centro-symmetric.

(ii) There are no translation vectors in reciprocal space.

(iii) The symmetry matrices in reciprocal space are the transposed inverses of the corresponding symmetry matrix in real space, i.e.

$$\text{if} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \underset{\sim}{M} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \text{ then } \begin{pmatrix} h' \\ k' \\ \ell' \end{pmatrix} = (\underset{\sim}{M}^{-1})^{T} \begin{pmatrix} h \\ k \\ \ell \end{pmatrix}$$

$\underset{\sim}{M}$ is usually a symmetry operator in one of the groups $\bar{1}$, 2/m, mmm, 4/m, 4/mmm, $\bar{3}$, $\bar{3}$m, 6/m, 6/mmm, m3 or m3m.

Input

1. TITLE; FORMAT(8A10)
   This will appear on the output and as a comment in the BLOCK DATA Subprogram.

2. NEQV; FORMAT(I5)
   This is the number of symmetry operation matrices (cards) which follow $0<NEQV\leq 24$

3. (A(I,J),I=1,3),J=1,3); FORMAT(9F3.0)

cc 1-3	a_{11}	elements in the real space symmetry operation matrix. (note: for programmers only) these elements are indexed as for a transposed matrix inside the program.
4-6	a_{12}	
7-9	a_{13}	
10-12	a_{21}	
13-15	a_{22}	
16-18	a_{22}	
19-21	a_{31}	
22-24	a_{32}	
25-27	a_{33}	

Up to 24 matrices may be input on cards 3.

Output

A. On paper the program lists the input matrix, its inverse, and the determinant of the input matrix.

B. To punch--a complete card deck, ready to be compiled, of BLOCK DATA SYMOPS.

Limitations

Only 24 matrices: this will be enough for all except for some cubic groups. For users in such dire predicaments their options are:

(i) re-dimension INVTRP, and SUBROUTINE SPACE in AVSORT

(ii) accomodate the missed symmetry element in the SUBROUTINE FORM they must write for AVSORT. Note that in this context the difference between 48 and 24 equivalent positions is only 1 symmetry operation and so the user need not become involved in a great deal of programming.

NAME: JIMDAP

CORE: 77K

AUTHOR: A. Zalkin-originally
Mods J. Ibers, F. Bernstein, G. Williams
DATE: November 1973

```
PROGRAM JIMDAP(INPUT,ØUTPUT,PUNCH.TAPE1,FØUR,TAPE3,TAPE11,TAPE5=INPUT,
               TAPE60=INPUT,TAPE6=ØUTPUT,TAPE61=ØUTPUT,TAPE4=PUNCH,
               TAPE20=FØUR,TAPE2=FØUR,TAPE45=TAPE11)
```

I. PURPOSE:

To calculate Fourier Synthesis.

II. TAPES:

A. FØUR-Binary Purpose-input data Format-JJ,KK,LL,sinθ/λ,FOBS,FC, cosα,sinα,ΔF,SIG

B. TAPE11-plot tape

III. LIMITATIONS:

IV. REPLACEABLE SUBROUTINES:

A. REJECT-used to reject reflections. Argument-NSKIP

B. IMP -data input other than FLINUS. Argument-JJ,KK,LL,AA,BB,IN

V. DECK SET UP

A. JOB CARD
1. TIME LIMIT - 1 minute for small maps
2. FIELD LENGTH - 77K
3. PRINT LIMIT - variable
4. NUMBER OF TAPES- 0-3
5. ECS - none

B. CONTROL CARDS

```
ATTACH(JIMDAP,JIMDAP,ID=CPRØGS)
REQUEST(FØUR,,,)
JIMDAP.
```

5

C. DATA CARDS:

CARD	FORMAT
1. Title card	6A10
2. Master control	(20I1,F10.4,I3)
3. Cell card	(6F9.6)
* 4. TRANS deck	SEE WRITE UP
5. RIP and SIG deck	
Card 1	5I5
Card 2	(9F5.5,5X,I3)
Card 3	3(F15.9,3I3)
* 6. Data cards	(3I9,2F9.5)
* 7. FRPLOT deck	(2I5,3F5.0,I5)

* MEANS OPTIONAL

Brookhaven Crystallographic Computer Program Writeup

NAME: JIMDAP FILES: 7 TIME: Variable

CORE FL: 77000

Purpose: Local version of the Zalkin Fordap program. It contains instructions which may be peculiar to the BNL CDC 6600 machine, and for this reason it may fail to operate on other systems without modification. In particular, the plotting packages may require some changes.

PRØGRAM JIMDAP(INPUT,ØUTPUT,PUNCH,TAPE1,FØUR,TAPE3,TAPE11,TAPE5=INPUT, TAPE60=INPUT,TAPE6=ØUTPUT,TAPE61=ØUTPUT,TAPE4=PUNCH,TAPE20=FØUR, TAPE2=FØUR,TAPE45=TAPE11)

JIMDAP consists of the following major subroutines:

RIP and SIG - routine for the calculation of the Fourier summation.

FRPRNT - routine for scaling and print-out of the Fourier summation in fixed point.

FRPEAK - routine for the location of peaks in the Fourier summation.

FRPLØT - routine for plotting the map, section by section, via the off-line Calcomp film and paper plotter. The plot is to scale.

TRANS - routine for the transformation of the data to enable sections in the Fourier summation to be calculated normal to a general vector.

Only those routines required for the particular job are called. Similarly, data input is required only for those segments which are called. The RIP-SIG segment writes the Fourier summation in binary on TAPE3. If a user tape was mounted at TAPE3 during the initial Fourier calculation, then the user tape can serve as an input tape for FRPRNT, FRPEAK, and FRPLØT in a subsequent run. TAPE11 is the tape written by JIMDAP for off-line plotting by the CRT and/or Calcomp plotter. FØUR is the binary input data tape read by JIMDAP and prepared by FLINUS. Input data may be on cards or in non-standard FØRMAT on tape or cards if the user supplies a special subroutine IMP.

Input Data:

Card A Title card (6A10); any desired Hollerith information.

Card B Master Control Card (20I1,F10.4,I3); (ISST(I),RMAX,NFILES)

col 1, ISST(1) = 0 no Fourier summation; do not call RIP - SIG.
= 1 calculate a Fourier summation; call RIP - SIG.

col 2, ISST(2)	= 0	no data transformation; do not call TRANS.
	= 1	TRANS is called and transformation matrix is supplied.
	= 2	TRANS is called and transformation matrix is determined from the equation of a general plane.
	= 3	TRANS is called and transformation is to a general plane perpendicular to a given vector.
	= 4	TRANS is called and transformation is to a general plane through three points.
col 3, ISST(3)	= 0	no printed output of Fourier summation.
	= 1	print the Fourier summation.
col 4, ISST(4)	= 0	no listing of peaks.
	= 1	search for and list peaks not on border.
	= 2	search and list peaks, including those on border.
col 5, ISST(5)	= 0	no plot tape written.
	= 1	write the plot tape. Supply TAPE11.
col 6, ISST(6)	= 2	double space FRPRNT output; any other digit, single space FRPRNT output.
col 7, ISST(7)	= 0	search for and list 1000 peaks (if present) in FRPEAK.
	= N	search for and list 100 *N peaks.
col 8, ISST(8)	= 0	no listing of unexpanded data;
	= 1	for listing of unexpanded data.
cols 9-10, ISST(9,10)	=	the number of columns of FRPRNT per page of output. If left blank the program sets this to 29, the maximum number allowed. If ISST(14) is non-zero then this is set to 50 if not otherwise specified. See below.
col 11, ISST(11)	= 0	normal
	= 1	punch peaks in FLINUS FØRMAT
col 12, ISST(12)		irrelevant
col 13, ISST(13)	= 0	no interpolation in peak search
	= 1	interpolate position of 150 highest peaks
	= 2	interpolate position and heights of 150 highest peaks
col 14, ISST(14)	= 0	normal FRPRNT output
	≠ 0	condensed plots suitable for teletype output. Letters A to T are used to represent the ranges 900 to 999, ... -900 to -999.
cols 15-20		no meaning now

cols 21-30, RMAX: This is the maximum scattering density of the map. It is determined by the scale of the input F values and the cell volume. If RMAX is read from this card as zero then the true RMAX is determined from the map by the program. Two reasons exist for inputting a value for RMAX here: (i) Some time may be saved if FPRNT or FRPLOT runs are submitted using a precalculated map on TAPE3; (ii) FRPRNT scales the output so that 999 is the largest value printed. The scaling constant C used for this is 999/RMAX. If it is desired that the output be some other multiple K of the scattering density then the value 999V/2K (where V is the unit cell volume) should be inserted here for RMAX. If the input data are on the absolute scale and RMAX is input here as zero then the true scattering density is given by

$$\rho_T = \frac{2}{V} \cdot \frac{RMAX}{999} \cdot R_{Printed} + \frac{F_{000}}{V}$$

where $R_{Printed}$ is the value which appears on the paper. The F_{000} term is not applied by the program.

cols 31-33, NFILES: # of files to be skipped on FØUR. Normally 0. If the FLINUS run included generation of both the FREDFUN (ØRFFE) and JIMDAP input files then set NFILES=1.

Card C Cell card (6F9.6); a, b, c, cosα, cosβ, cosγ

Cards D TRANS deck (supplied only if ISST(2)≠0)

Option 1: (ISST(2)=1). Transformation matrix is supplied. The subroutine will determine cell constants for a new pseudo cell, print out the transformation information, and return the determinant of the transformation matrix to the main routine.

card 1 9F8.4 $U_{11}, U_{12}, U_{13}, U_{21}, U_{22}, U_{23}, U_{31}, U_{32}, U_{33}$, the elements of the transformation matrix, where ANEW=U*AOLD.

card 2 must be a blank card.

Option 2: (ISST(2)=2). Transformation matrix is determined from the equation of a general plane. New axis 1 is normal to this plane, axes 2 and 3 are in the plane. The lengths of these axes are determined in the following way:

For each axis, consider the following four quantities:

(1) 10.0 Angstroms
(2) 2.0 * XMAX(I) (in Angstroms)
(3) 2.0 * XMIN(I) (in Angstroms)
(4) Cell(I), where I is the number of the axis

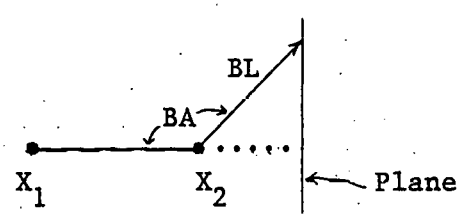
The length of axis I is set to the maximum of these four quantities. The purpose of specifying a large CELL(I) (below) is to obtain higher accuracy in the fitting of a non-rational plane. This causes an increase in storage requirements and in computation time, however.

Input cards for this option are as follows:

card 1 FØRMAT(7F10.5,3F3.3)
P1,P2,P3,D,CELL(1), CELL(2), CELL(3), XI(1), XI(2), XI(3)
Equation of the plane in the form P1 X + P2 Y + P3 Z = C.
(CELL(I),I=1,3) as described above.
(XI(I),I=1,3) Position in triclinic coordinates of a point to which the limit information on card 2 is applied.

card 2 FØRMAT(9F8.4) XMIN, XMAX, YMIN, YMAX, ZMIN, ZMAX, DELX, DELY, DELZ.
Limit and increment information, in angstroms in directions of new axes. These quantities are added on to the point corresponding to the coordinates XI(I) entered on card 1. If XMIN = XMAX, the program assumes that the only section to be calculated is the plane parallel to the one specified on card 1 at a distance XMIN = XMAX from it. Thus, for a Fourier in the specified plane, always set XMIN = XMAX = 0. But do not set DELX=0.

Option 3: (ISST(2)=3) Given two points X1 and X2, a bond length BL and bond angle BA, a plane is calculated which is perpendicular to the vector X2-X1 and is a distance -BL COS(BA) from X2:



card 1 FØRMAT(8F10.4) (X1(I),I=1,3),(X2(I),I=1,3),BL,BA
The coordinates of the atoms are in the triclinic fractional coordinates. BL is in angstroms, and BA is in degrees.

card 2 FØRMAT(3F10.5) (CELL(I),I=1,3) as described above.

card 3 FØRMAT(9F8.4) Limit card in angstroms as described above (card 2, option 2)
The origin is taken at the point where the vector X2-X1 intersects the plane.

Option 4: (ISST(2)=4) A plane is calculated which includes the three points X1, X2, and X3.

card 1 FØRMAT(9F5.4) (X1(I),I=1,3),(X2(I),I=1,3),(X3(I),I=1,3)
coordinates of the three points in the triclinic cell.

card 2 Same as for option 3.

card 3 Same as for option 3. The origin is assumed to be at the midpoint of the three points.

N.B. The TRANS deck must be submitted and called if FRPEAK, FRPLØT are to be performed in a separate job from the one in which tape 3 was written by RIP and SIG.

Cards E RIP (and SIG) deck (supplied only if ISST(1)≠0)

card 1 6I5 NEQUIV,NREF,NTAPIN,NONTAP,NREJ

NEQUIV - the number of equivalent positions for the space group, not including translational or symmetry centers.

Laue group	NEQUIV	Laue group	NEQUIV
$\bar{1}$	1	$\bar{3}$	3
2/m	2	$\bar{3}$m	6
mmm	4	6/m	6
4/m	4	6/mmm	12
4/mmm	8	m3	12
		m3m	24

NREF - the number of expanded data sets to be listed. RIP expands the non-equivalent reflections into the corresponding equivalent reflections (not related by a center). This listing provides a convenient check on the program and user. It does use up paper, however, so it is generally advisable to expand a limited number of reflections, advisably including some general reflections.

NTAPIN - code word to indicate source of data and calculation desired

0 if data are from cards or as defined in subroutine IMP

The following cases are for FØUR written by FLINUS with F (NOT F**2) on it

20 compute difference Fourier
21 compute difference Fourier but delete terms for $F_{obs}=0$
22 compute Fourier using F_{obs} with phases from F_{calc}
23 compute Fourier based on F_{calc}
24 compute Patterson from OBS
25 compute Patterson from CALC
26 compute alpha synthesis:

```
A=OBS**2*CALC*COSalpha
B=OBS**2*CALC*SINalpha
```

α = phase angle

Note well: For a FØUR tape from FLINUS with F**2 on it (i.e. refinement on F**2) options 20 through 26 are obtained by making NTAPIN 120 through 126. In this case, all non-positive F^2 are rejected.

For input out of XDATA (which produces F^2 and modified F^2 on tape), 20 corresponds to an origin-removed Patterson, 22 ordinary Patterson, 23 a sharpened Patterson.

100 calculate Patterson from F^2 on tape, but delete reflections with negative F^2 values.

NØNTAP 0 the first 10000 data are used in the summation
non-zero: use only the first NØNTAP data in the summation

NREJ 0 no special reject subroutine is called
1 call subroutine REJECT (NSKIP)
This subroutine, as written by the user to replace the dummy supplied with the program, can be used to reject certain reflections. See page 8.

card 2 limit and direction card FØRMAT(9F5.5,5X,I3) Triclinic coordinates.
XMIN,XMAX,YMIN,YMAX,ZMIN,ZMAX,DELTAX,DELTAY,DELTAZ,NØRIEN

where the summation goes, for example, from XMIN to XMAX in steps of DELTAX, YMIN to YMAX in DELTAY, etc. NØRIEN is 100, 10, 01 for sections perpendicular to a, b, c, resp. The map orientations defined by NØRIEN ARE:

NØRIEN	HØRIZ	VERT	SECT
100	z	y	x
10	x	z	y
1	x	y	z

The program is so designed that if one wants to run over an entire cell, for example, in the x direction, then run from -0.5 to 0.5, not from 0 to 1.0. If the user is inhibited by this apparently capricious restriction then he/she may indulge in whatever cell interval desired simply by supplying a dummy SUBRØUTINE CHEKUP in place of the one provided. There are no restrictions on the intervals, other than those imposed by the format. Thus one can run from -0.40000 to 0.0 in steps of 0.00125.

card 2 is not relevant if TRANS, options 2, 3 or 4, is called.
In this case card 2 must be resubmitted, but may be blank.

Despite the above flexibility it is still sometimes difficult to arrange true-to-scale maps which begin and end exactly at the desired fractional cell coordinates. If the cell grid increments DX, DY, DZ are set to values greater than 1.0 then the program will redefine each of these quantities independently by a Fortran statement of the form

```
IF(DX.GT.1.0)   DX = ABS(XMAX-XMIN)/DX   .
```

Note that in this case the effective grid interval is dependent upon the unit cell interval, also note that only when whole number values of DX etc. are specified is this facility of optimum usefulness.

cards 3 NEQUIV equivalent position cards 3(F15.9,3I3)
The format here is identical with that used for symmetry cards in FLINUS, ØRFFE, etc. and is

cols	1-15	translational part of transformed x
	16-18	multiplier of x
	19-21	multiplier of y
	22-24	multiplier of z
	25-39	translational part of transformed y
	40-42	*x
	43-45	*y
	46-48	*z
	49-63	translational part of transformed z
	64-66	*x
	67-69	*y
	70-72	*z

Thus for the unlikely symmetry equivalent position 2/3 - x, y - 2z, $\bar{x}$, we would have in the appropriate format:

0.6666667 -1 0 0 0.000000 0 1 -2 0.000000 -1 0 0.

NOTE: The NEQUIV symmetry elements plus the center of symmetry (if one is present) must reproduce all equivalent positions in the space group, with the exception of lattice centering.

Cards F Reflection data cards (if NTAPIN is 0)
h,k,ℓ,AA,BB (real and imaginary parts of structure factor) are read via the replaceable subroutine IMP. The IMP routine is as follows:

```
      SUBRØUTINE IMP(JJ,KK,LL,AA,BB,IN)
      READ(IN,230)  ISENT,JJ,KK,LL,AA,BB
  230 FØRMAT(I1,I3,2I4,2F9.3)
      IF(ISENT.EQ.1) JJ=999
      RETURN
      END
```

The input may be terminated either by ISENT=1 or JJ=999, but in either case JJ must be returned as 999 for JIMDAP to work properly. IN is the number of the system input file (currently 5 and 60). For example, if one wishes to read reflection data from the AVSØRT BCD output tape in order to calculate a Patterson, one could request the tape by the name FØUR (which is equivalenced to TAPE20 on the program header card) and replace IMP by

```
      SUBRØUTINE IMP(JJ,KK,LL,AA,BB,IN)
      READ(20,230) ISENT,JJ,KK,LL,AA
      BB=0.0
      IF(ISENT.EQ.1) JJ=999
      RETURN
  230 FØRMAT(I1,F3.0,2F4.0,F9.3)
      END
```

NOTE: Input data for FRPRNT and FRPEAK are covered in the SETUP deck and no special data decks are required. Some remarks about these routines are:
FRPEAK will work on three or more sections. If it is set up to ignore peaks on the borders, then it is possible in the limit card in RIP to run in x, say, from -0.02 to 0.52 in steps of 0.02 as a check on symmetry, and yet not get extra peaks. In addition to the location of the peak, to the nearest grid point, FRPEAK also finds the height and lists this also in absolute units of e/A^3, if the data are scaled in electrons and if the calculation is a Fourier. There are now options (see card B) for interpolation and border peaks.

Card G FRPLØT deck (supplied only if ISST(5)≠0)

card 1 FØRMAT(2I5,3F5.0,I5) (NSEC,NSKIP,CMAX,CMIN,CINT,ILN)

NSEC = 0 for projections (does some scaling of axes best understood by reading the program)
= 1 for sections

NSKIP number of sections to be skipped before plotting

CMAX the maximum contour level to be plotted on the scale of FRPRNT. Thus CMAX=1000 will plot to the top of the highest peak on the FRPRNT output.

CMIN the minimum contour level on the same scale. CMIN can be negative.

CINT the contour interval on the same scale.

ILN = 0 normal operation
= 1 eliminate grid lines and border from plot.

After the calculation, the user TAPE11 is submitted for off-line CRT and/or Calcomp plotting simply by completing the Calcomp request form available at the Chemistry Department or the Computing Center. Generally, it is quickest and most convenient to have only the CRT plot made. The resulting 35 mm film can be enlarged to 8½ x 11".

Replaceable Subroutines

SUBRØUTINE REJECT (NSKIP)

COMMON/R/JJ,KK,LL,SINL,FOSV,FOBS,SFSV,SFCALC,DELSV,DEL,COSAA,SINAA, AA,BB,SIG

This routine is called (if NREJ.NE.0) from RIP after the various options of NTAPIN have been exercised, but before the reflection is used in the calculation. To keep the reflection, return with NSKIP=0; to reject the reflection, return with NSKIP≠0.

In COMMON JJ,KK,LL are the indices.

If input is from FLINUS SINL is $\sin\theta/\lambda$.

FOSV, SFSV, DELSV are the input values of FOBS, SFCALC, DEL if NTAPIN GT 100. Otherwise these are not defined.

FOBS, SFCALC, DEL are the input values if NTAPIN LT 100.
If NTAPIN GT 100 then these are related to the above quantities by

FOBS = SQRT(FOSV), SFCALC = SQRT(SFSV) DEL = FOBS - SFCALC

COSAA, SINAA are the cosine and sine of the phase angles.

AA and BB have been defined above. Any modification of actual Fourier calculations must involve changes in AA and BB at this point. Changing the sign of both AA and BB will change the sign of the map. This is useful, since it allows the peak-picking algorithm to be used to search for negative peaks (e.g. those from hydrogen atoms in neutron diffraction).

SIG is the SIG on the structure factor printout from the least-squares (i.e., the original SIG modified by the WEIGHT routine and possibly by the scale factor).

If NTAPIN = 0 (card or special input) then only JJ,KK,LL,AA,BB are available here.

SUBRØUTINE IMP (JJ,KK,LL,AA,BB,IN)

see description under cards F on page 7.

Tapes

FØUR

JJ,KK,LL,sinθ/λ,|FØBS|,|FCALC|,COSα,SINα,ΔF,σ

one binary record per reflection.
Terminated by end-of-file, not JJ=999.

TAPE3 Intermediate tape holds Fourier synthesis. Buffered in 1600 word binary records. See listing for details. Cannot be read by the old routine FØRDAP.

TAPE1 A scratch file used by the program.

Further notes

(1) In some large problems, storage requirements may split each section into several parts. A routine GATHER is available to assemble these into single sections for plotting.

(2) The user should usually supply a TAPE3. If program is interrupted while printing or plotting, TAPE3 may be used to reinitiate. Much time may be saved in such a case.

Brookhaven National Laboratory
Chemistry Department

CRYSNET Program Writeup

CDC CYBER 70/74,CDC CYBER 70/76
CDC SCØPE 3.4, CDC SCØPE 2.1

```
PRØGRAM LEASTSQ(DATA,FØUR,PUNCH,INPUT,ØUTPUT,
*TAPE1,TAPE2,TAPE3,TAPE4,
*TAPE20=FØUR,TAPE14=DATA,TAPE5=INPUT,
*TAPE6=ØUTPUT,TAPE7=PUNCH)
```

Purpose: A least squares program to refine heavy atom parameters in an isomorphous series and to include molecular refinement phase information.

Introduction: This program was written by M. G. Rossmann of Purdue University and modified by Alan Wonacott, Margaret Adams, Geoffrey Ford (Purdue), Gary Quigley, Byron Rubin, Sung Hou Kim (Duke), Herbert Bernstein (Brookhaven).

The program follows the ideas of Blow, D. M. and Crick, F.M.C., Acta Cryst., 1959, 12, 794; Dickerson, R. E., Kendrew, J. C., and Strandberg, B. E., Acta Cryst., 1961, 14, 1188; Dickerson, R. E., Kopka, M. L., Varnum, J., and Weinzierl, J. E., Acta Cryst., 1967, 23, 511; and North, A.C.T., Acta Cryst., 1965, 18, 212.

Input data:

I. CDC 7600 Input stream cards

This is, at present, the general run stream of cards for use on the CDC 7600 at BNL. The cards required by the program are under the control of an Editor subroutine. N.B. Do not include blank cards in this deck except in the places indicated.

1. XI, CP7Ø, YD1, T3ØØ. Name.

2. ACCOUNT (PROTEIN,331) put in your own account card

2a. REQUEST (PUNCH,*PF) Request for permanent file PUNCH (for example) to be open during run.

3. MOUNT (VSN = CHEM Ø1, SN = CHEM)

4. ATTACH (LGO, LEASTSQ, ID = XHJB, SN = CHEM)

5. MODE (Ø)

6. ATTACH (PTCMER, PTCMER, ID = XHJB, SN = CHEM)

   This is a MERGEL output file read in from PDP-11

7. ATTACH (EDIT, EDIT, ID = CPROGS)

8. COPYBF (PTCMER, CCD)

9. EDIT (INPUT,CCD, ,OUTPUT) This merges MERGEL data with control cards.

10. LDSET (PRESET = ZERO)

11. LGO (,,, CCD)

12. EXIT

12a. CATALOG (PUNCH, PUNCH, ID = PROTEIN, RP = 999) RP = retention period (3 days if not used is maximum)

13. DMP (3ØØØØ)

14. 7/8/9 EOR card

15. 8Ø, } For Editor subroutine

16. M

*17. IOSET data card

18. blank

19. EM part of Editor

20. ØØØØØØØØØterminator card

    N.B. Do not put in 7/8/9 EOR at this point since data cards are actually being edited in

21-36. At this point include cards required by the program. See II, starting page 3.

37. blank card

38. blank card

39. PQ

    in cols 1,2

40. DEC EOF card

*IOSET card is described under II, page 3.

II.

*17 IOSET Control Card

(BNL I/O adapted from Duke I/O adapted from Purdue)

This card controls the various tapes required by the LEASTSQ PROGRAM

IIN, IOUT, INCARD, IOUT1, IOUT2, IOUT3, IOUT4, MMM 815

The files listed in the program itself are:

LEASTSQ (DATA, FOUR, PUNCH, INPUT, OUTPUT, TAPE1, TAPE2, TAPE3, TAPE4, TAPE20 = FOUR, TAPE14 = DATA, TAPE5 = INPUT, TAPE6 = OUTPUT, TAPE7 = PUNCH)

col 5	IIN	Any integer. This is set by the program to 14 (=DATA) if tape input of data, 2 if card input of data. Tape input read into IIN.
col 10	IOUT	Any integer, set by program to 7 (=PUNCH). If 0, no assignment and write on IOUT statements ignored. Used for tape output. (TAPE7 = IP = PUNCH) will receive a coded file which may be used for a map of the native protein if IOUT ≠ 0.
col 15	INCARD	1 Reflection data on cards (read into TAPE5 = INPUT) 0 Reflection data on tape (IIN = TAPE14 = DATA)
col 20	IOUT1	0 no assignment. Ignore write IOUT1 statements. 1 or any integer. Program sets this to 1 (=TAPE1).
col 25	IOUT2	0 no assignment. Ignore write IOUT2 statements. 1 or any integer. Program sets this to 2 (=TAPE2).
col 30	IOUT3	0 no assignment. Ignore write IOUT3 statements. 1 or any integer. Program sets this to 3 (=TAPE3).
col 35	IOUT4	0 no assignment. Ignore write IOUT4 statements. 1 or any integer. Program sets this to 4 (=TAPE4)
col 40	MMM	Write out data on IOUT4 for heavy atom derivative if that derivative is numbered MMM.

Control information, i.e. cards 21-36 of input stream, is read onto INPUT (TAPE5).

If data are included on OUTPUT (TAPE6) they are copied to TAPE2 for use as binary input.

If data are on a separate binary file, they should appear on DATA (TAPE14).

On the first cycle, binary data for the next cycle are written on TAPE1.

On the next cycle TAPE1 will be read and TAPE2 written, etc.

A binary file which may be used for maps is written on FOUR (TAPE20).
N.B. CARDIN, TAPEIN and TAPOUT can be modified. MODIFY is used, for example, to reject a reflection containing bad data.

Reflection Data Input

Data should be on an absolute scale or F_P modified by SCALE and F_{PH} modified by SCL. The data may be formatted ("cards") or binary ("tape").

a) Card input

If on "cards" the following format is expected.

Format 3I3, 2F6.2, I2, 2X, 3F6.2, I2, 2X, 3F6.2, I2

IH, IK, IL, FNAT, ERNAT, NNAT, (F(II),AD(II),ERR(II), NNHV(II), II = 1,2)

$$\left.\begin{array}{l} IH = \\ IK = \\ IL = \end{array}\right\} h,k,\ell$$

FNAT = F native = F_P

ERNAT = error in F native, e.g. $\sigma(F)$

NNAT = 0 for observed, 1 for unobserved

F(1) = F for compound 1 = F_{PH1}

AD(1) = anomalous dispersion for compound 1 = $F^{+}_{PH1} - F^{-}_{PH1}$

ERR(1) = error in F for compound 1 = σF_{PH1}

NNHV(1) = 0 for observed, 1 for unobserved

F(2) = F for compound 2 = F_{PH2}

AD(2) = anomalous dispersion for compound 2 = $F^{+}_{PH2} - F^{-}_{PH2}$

ERR(2) = error in F for compound 2 = σF_{PH2}

NNHV(2) = 0 for observed, 2 for unobserved

If you wish to change the card input then you may insert the replaceable subroutine CARDIN.

```
SUBROUTINE CARDIN (unit, NNO, IH, IK, IL, NNAT, FNAT, ERNAT, ADNAT, FAZBST,
                   FAZMP, FIGMER, NNHV, F, ERR, AD)

     DIMENSION NNHV(8), F(8), ERR(8), AD(8)
```

b) Tape input

If the input reflection data are in binary form the following format is expected by the program.

IIN = input tape = 14 = DATA (This is not on the reflection data tape.)

NNO = sequence number = # of reflection (1,2, etc.). 0 for end of data. -1 for discard.

IH = h
IK = k
IL = ℓ
} integer indices

NNAT = 0 for unobserved, n for observed in crystal n (1 for native, but see below)

FNAT = native F

ERNAT = σ(native F) = error in native F

ADNAT = anomalous dispersion for F native = $F^+ - F^-$

FAZBST = best phase (radians)
FAZMP = most probable phase (radians)
FIGMER = figure of merit
} initialized in the program if CARDIN is used

NNHV(II) = 0 for compound unobserved, n for observed in crystal n (each atom with its own temperature factor)

F(II) = heavy atom derivative II = F_{PHII} (II = 1 to 8 maximum)

ERR(II) = error in F for heavy atom derivative II

AD(II) = anomalous dispersion for F for heavy atom II

Terminator is EOF on tape

The format of binary data files DATA, TAPE1, TAPE2 may be altered by altering the subroutine TAPEIN for reads and TAPOUT for writes. TAPEIN calls MODIFY which is a dummy routine which may be used to discard or modify data.

TAPEIN has the same arguments as CARDIN.

Cards that remain the same during successive refinement cycles.

21. Title card Format 20A4 TITLE (I), I = 1,20

22. Cell dimension card Format 9F8.0

(RECIP(K), I = 1,6), DSTMAX, DSTMIN, GAP

cols 1-8	a, or a^{*2}	units of Å, $Å^{-2}$ or degrees
9-16	b, or b^{*2}	
17-24	c, or c^{*2}	
25-32	cosα, α, or 2a*b*cosγ*	
33-40	cosβ, β, or 2b*c*cosα*	
41-48	cosγ, γ, or 2c*a*cosβ*	
49-56	DSTMAX ($\frac{1}{dmin}$ or d*max)	units of $Å^{-1}$
57-64	DSTMIN ($\frac{1}{dmax}$ or d*min)	
65-72	GAP $\frac{1}{dgap} = \frac{1}{\Delta d} = \frac{\Delta d^*}{\lambda}$	

Used to divide up results into shells. If GAP = 0 it is automatically set equal to 0.1/1.5418.

23. Refinement information card

Format 4I5, 4F10.4, I5

NSYM, NCPDS, IANGLE, NCYCLE, SCALE, FIGMIN, FGAP, REJANO, IFPRNT

cols 1-5	NSYM = number of symmetry cards
6-10	NCPDS = number of heavy atom compounds to be refined
11-15	IANGLE = angular increment in degrees to be used in estimating the phase probability distribution = Δα
16-20	NCYCLE = number of cycles to be executed
21-30	SCALE = scale factor to be applied to structure amplitudes of native protein. This is not varied during the program.
31-40	FIGMIN = any reflection whose phase is determined with a figure of merit less than FIGMIN will have extra information on output.
41-50	FGAP = integral ranges of |F| for dividing up results into shells.
51-60	REJANO = filter for anomalous dispersion. If AD > REJANO, ignore the result. This eliminates certain kinds of errors but does not filter the native data.
65	IFPRNT = 0 no print, 1 print, 2 print input data as well.

24. Magnifications

Format 8 F10.3

AMAGS, AMAGBO, AMAGA, AMAGX, AMAGY, AMAGZ, AMAGB

cols 1-8 AMAGS = multiplier for Δ (scale)

9-16 AMAGBO = multiplier for Δ (overall B)

17-24 AMAGA = multiplier for Δ (occupancy)

25-32 AMAGX =
33-40 AMAGY = } multiplier for Δx, Δy or Δz
41-48 AMAGZ =

49-56 AMAGB = multiplier for ΔB

These values magnify or modify the appropriate calculated shifts and are only used in the final output step.

25. Compound card - identification on "F input tape"

Format 8I3

NFS(I), I = 1,8

cols 1-3 NFS(1) = column on "F input tape" designated "compound 1"

4-6 NFS(2) = column on "F input tape" designated "compound 2"

---- NFS(NCPD) = column on "F input tape" designated "compound NCPD"

This allows some flexibility in working with a given input tape.

26. NPCYCL

Format I6I5 1 in each entry position. (May not work properly with any other entry.)

This was included to allow a variation of the number of cycles of least squares relative to the number of cycles of Phase (cf. Muirhead).

27. Symmetry cards

Format 12F3.0 (T(N,I,J), J = 1,4), I = 1,3) N = 1, NSYM

These are NSYM cards, one card per symmetry position (see International Tables).

cols 3, 6, 9, 10-12, 15, 18, 21, 22-24, 27, 30, 33, 34-36

t_{11}, t_{12}, t_{13}, t_{14}, t_{21}, t_{22}, t_{23}, t_{24}, t_{31}, t_{32}, t_{33}, t_{34}

If a point in the first asymmetric unit is at x_1, y_1, z_1, then a point in the nth asymmetric unit will be at

$$x_n = t_{11}x_1 + t_{12}y_1 + t_{13}z_1 + t_{14}$$

$$y_n = t_{21}x_1 + t_{22}y_1 + t_{23}z_1 + t_{24}$$

$$z_n = t_{31}x_1 + t_{32}y_1 + t_{33}z_1 + t_{34}$$

There must be as many symmetry cards as there are asymmetric units in the unit cell

For example I222 8 cards

1	0	0	.0	0	1	0	.0	0	0	1	.0
-1	0	0	.0	0	-1	0	.0	0	0	1	.0
1	0	0	.0	0	-1	0	.0	0	0	-1	.0
-1	0	0	.0	0	1	0	.0	0	0	-1	.0
1	0	0	.5	0	1	0	.5	0	0	1	.5
-1	0	0	.5	0	-1	0	.5	0	0	1	.5
1	0	0	.5	0	-1	0	.5	0	0	-1	.5
-1	0	0	.5	0	1	0	.5	0	0	-1	.5

Cards that are changed during refinement

At the end of the requested number of refinement cycles new cards are punched. These can replace previous cards of this type, and are ready for further refinement on resubmitting the deck.

28. Error as a function of F native

8F8.1 (FSIZE (J,2), J = 1,8)

cols. 1-8 FSIZE(1) = r.m.s. lack of closure error for reflections $0 \leq |F| < F_{GAP}$

9-16 FSIZE(2) = r.m.s. lack of closure error for reflections $F_{GAP} \leq |F| < 2F_{GAP}$

57-64 FSIZE(8) = r.m.s. lack of closure error for reflections $7F_{GAP} \leq |F|$

Should be of the order of $\sigma(F)$. N.B. in F_{GAP} (not d_{GAP}) units. $\sigma(\underline{F}) \sim 0.07\ \underline{F}$

K. Cards for each compound

Cards for "compound 1" are first and so forth according to allocations in "compound card" (25, above). The cards are repeated for each derivative. There are NCPDS sets of cards, i.e. (30 through 36) x NCPDS. I is the number of NCPDS under consideration.

29. Compound property card

Format 2I5, F10.5, 2A4

NATOM(I), NCRYST(I), CAY(I), CPDTLE(I,1), CPDTLE(I,2)

cols 1-5 NATOM = number of heavy atoms in this derivative, i.e. number of sites for this one heavy atom.

6-10 NCRYST = identifier of crystal. List every crystal to be refined separately on a separate card.

11-20 CAY = $\Delta f''/(f + \Delta f')$ for defining the size of anomalous dispersion. If CAY is zero, it is assumed that there are no anomalous dispersion observations. If CAY is negative, the hand of the heavy atom is changed. (CAY = 0.107 for Hg). Values are computed for $(\sin\theta/\lambda) = 0.0$.

21-24 CPDTLE(1) =
25-28 CPDTLE(2) =
} Title (8 positions)

30. Isomorphous error card

Format 8F8.1

EIS (I,J), J = 1,8

cols 1-8 EIS(1) = r.m.s. lack of closure for this compound in range $0 \leq 1/d < GAP$

9-16 EIS(2) = r.m.s. lack of closure for this compound in range $GAP \leq 1/d < 2GAP$

57-64 EIS(8) = r.m.s. lack of closure for this compound in range $7GAP \leq 1/d$ (r.m.s. lack of closure for this compound in the range $(J-1) \times GAP \leq 1/d < J \times GAP$). ($d_{GAP}$ units. Should be of the order of $\sigma(F)$.

31. Anomalous dispersion error card

Format 8F8.1

EAD(I,J), J = 1,8

cols 1-8 EAD(1) = r.m.s. differences between observed and calculated anomalous dispersion in range $0 < 1/d < GAP$.

9-16 EAD(2) = ditto for $GAP \leq 1/d < 2GAP$

57-64 EAD(8) = ditto for $7GAP \leq 1/d$ (r.m.s. difference between observed and calculated anomalous dispersion in the range $(J-1) \times GAP \leq 1/d < J \times GAP$). These can be determined from anomalous differences of centric vs noncentric reflections. (d_{GAP} units. Should be of the order of $\sigma(F)$.

32. Card for each crystal

There are M = NCRYST(I) cards, one for each crystal of the given compound, i.e. each data set.

Format I5, 2F10.4, I5

J is the number of the particular heavy atom under consideration

NZ(I,J), SCL, BOVER(I,J), IFBOVR(I,J)

col 5 NZ = number that has to match the identifier NNHV on tape. It must match the observed flag.

6-15 SCL = scale to apply to F_{PH} values for this compound after scale has been applied to FNAT. This is the scale that is REFINED in this program. N.B. SCALE (applied to F_P) is <u>not</u> refined in this program.

16-25 BOVER = overall B to apply to F values for this compound. This is generally set equal to zero.

30 1 if overall B to be refined

0 if overall B not to be refined

33,34,35. <u>Three cards for each atom</u>

J is the number of the atom under consideration. There are 3 x NATOM cards, i.e., occupancy, coordinate and temperature factor cards, 33, 34, 35.

1. <u>Occupancy of atom LIST</u>

Format 8F10.4 ANUM (LIST, K), K = 1,M

cols 1-10 ANUM (1 per crystal) atom number or occupancy card (atomic number) for the heavy atom

11-20 etc. If there are M crystals of a given heavy atom derivative type with the <u>same</u> heavy atom position then there should be M values of ANUM, reflecting different occupancies in different crystals.

2. <u>Coordinate cards</u>

Format 3F10.4, I5, 5X, 5I1

X(LIST), Y(LIST), Z(LIST), NTROP(LIST), (LABEL(LIST, K), K = 1,5)

cols 1-10 X =
11-20 Y =
21-30 Z =
} fractional positional parameters for heavy atom

35 NTROP = 1 = isotropic shape parameter
6 = anisotropic shape parameter

41 LABEL(1) = controls atomic number refinement
42 LABEL(2) = controls x refinement
43 LABEL(3) = controls y refinement
44 LABEL(4) = controls z refinement
45 LABEL(5) = controls shape parameter refinement
} 0 = no refinement, 1 = refinement — Refinement flags

3. <u>Temperature factor cards</u>

cols 1-10 Format 6F10.6 (BLIST,K), K = 1,6

B for an isotropic atom. Shape factor is $\exp(-B\frac{\sin^2\theta}{\lambda^2})$.

β_1, β_2, β_3, β_4, β_5, β_6 for an anisotropic atom. Shape factor is $\exp(-(h^2\beta_1 + k^2\beta_2 + \ell^2\beta_3 + hk\beta_4 + k\ell\beta_5 + \ell h\beta_6)$.

Total temperature factor = BOVER + B(LIST, K).

OUTPUT Values in parentheses are computed by the program.

A. First page (Main program) (This page is a relisting of input data)

1. Title for problem (TITLE(I), I = 1,20)

2. MAGNIFICATION FACTORS FOR SHIFTS ARE

   FOR SCALE (AMAGS)

   FOR BOVER (AMAGBO)

   FOR ANUM (AMAGA)

   FOR X, Y, Z (AMAGX,AMAGY,AMAGZ)

   FOR B (AMAGB)

3. RECIP = RECIP(1) to RECIP(6)) a^{*2} b^{*2} c^{*2} $2a^*b^*\cos\gamma^*$ $2b^*c^*\cos\alpha^*$ $2c^*a^*\cos\beta^*$

   DSTMAX = (DSTMAX) DSTMIN = (DSTMIN) GAP = (GAP) d^*max d^*min gap

4. NSYM = (NSYM) NCPDS = (NCPDS) IANGLE = (IANGLE) NCYCLE = (NCYCLE) n_s n_{cpd} $\Delta\alpha_i$ n_{cycl}

   SCALE = (SCALE) FIGMIN = (FIGMIN) FGAP = (FGAP) REJANO = (REJANO) IFPRINT = (IFPRNT)

5. NPCYCL = NPCYCL(1) to NPCYCL(16))

6. SYMMETRY CARDS

   (((T(N,I,J),J=1,4)I=1,3)N=1,NSYM) t_{ij}

   One line per asymmetric unit

7. FSIZE = (FSIZE(J,2),J=1,9) Er_1 to Er_8

B. New page, one for each derivative (Main program). (I = 1,NCPDS)
   (Much of this page is also a relisting of input data)

1. Title for problem (as on first page) (TITLE(I), I=1,20)

2. COMPOUND (I) (CPDTLE(I,1),CPDTLE(I,2))

   NATOMS = (NATOM(I)) n_{HAl}

   NCRYST = (NCRYST(I)) n_{cryst}

   CAY = (CAY(I)) cay

3. EIS = (EIS(I,J),J=1,8) $E_{IS1} \cdots\cdots E_{IS8}$ = errors in isomorphous measurements

   EAD = (EAD(I,J),J=1,8) $E_{AD1} \cdots\cdots E_{AD8}$ = errors in anomalous dispersion measurements

4. One set for each heavy atom derivative (J=1,M(M=NCRYST(I)))

   CRYSTAL NO. (J) NZ(I,J)= (NZ(I,J))

   SCALE = (SCL) k_2

   BOVER = (BOVER(I,J)) IFBOVR = IFBOVR(I,J)) Bov

5. One for each atom (J=1,N(N=NATOM(I,J))

   ANUMS = ((ANUM(LIST,K),K=1,M) Z

   COORDINATES = (X(LIST),Y(LIST),Z(LIST) x y z

   NTROP = (NTROP(LIST), (B(LIST,K),K=1,6)) NTROP β_1 to β_6

   LABEL = (LABEL(LIST,K),K=1,5) LABEL = flags for refinement

6. END OF FILE ENCOUNTERED AFTER REFLECTION (H(II2),II2=1,3)

7. ZERO CORLAT (M,N) (M=1,NVAR, N=1,NVAR)

   Row and column of correlation matrix where

   NVAR = number of variables

   This is printed if CORLAT(M) =0, i.e. there is a zero entry in a diagonal term of the correlation matrix

   ERROR AFTER REFLECTION (H(II2),II2=1,3)

   Message printed if NNHV(MPCD) does not equal any NZ(M,K1)

C. Next page (Main program)

1. Title for problem (as on first page) (TITLE(I), I=1,20)

2. CORRELATION MATRIX

   (CORLAT(N),N=1,NVAR) 10 per line maximum

   If the elements of the least squares matrix are a_{ij}, then the elements of the correlation matrix are $\frac{a_{ij}}{\sqrt{a_{ii}a_{jj}}}$.

   Since this is a symmetric matrix all elements with $i > j$ are set to zero. Each row of n of the matrix is printed out in a series of 10 elements per line For instance, if there are 42 parameters under refinement there will be 42 elements per row. Each row is printed out as 4 lines of 10 numbers and one line of two numbers.

D. New page. (Phase program) Continuous for all reflections

1. (IH,IK,IL,FP,ABEST,AMAX,FBEST,(M,FH(M,1),FH(M,3),FH(M,2)PHI(M),REAL(M),EMAG(M)) for M=1,MCPDS.

2. (H(J),J=1,3) FNATIVE = (FP) FIG OF MERIT = (FBEST) BEST AND MOST PROBABLE

PHASES ARE (A1) ϕ_{best} (A2) ϕ_{max}

3.	CPD	FH	AD	FSMALL	PHI	A	B
	HA number	F_{PH}	$F^{+}_{PH}-F^{-}_{PH}$	$fj=F_{HA}$ only	α_{HA}	A_{HA}	B_{HA}
4.	(M)	(FH(M,1))	(FH(M,3))	(FH(M,2))	(PHI(M))	(REAL(M))	(EMAG(M))

5. TOTAL PHASE PROBABILITY CURVE

6. (P(J),J=1,JJ2)

7. (P(J),J=JJ2,JJ,P(1))

$\left(\frac{P(\alpha)}{P(\alpha)_{max}}\right)$ in intervals $\Delta\alpha_i$ from 0-180° and from 180°-360°. The probabilities of $P(\alpha)$ at a given phase α used in computing the figures of merit are computed. Increments, $\Delta\alpha$, are input in card 23 as IANGLE. The equation, for N heavy atoms, gives a probability $P(\alpha)_h$ for each reflection h:

$$P(\alpha)_h = \prod_{i=1}^{N} \exp\left(-\frac{\varepsilon^2_{isi}}{2E^2_{isi}}\right) * \prod_{i=1}^{N} \exp\left(-\frac{\varepsilon^2_{adi}}{2E^2_{adi}}\right)$$

where $\varepsilon_{is} = |F_{PHobs} - F_{PHcalc}|$

and $\varepsilon_{ad} = |AD_{obs} - AD_{calc}|$

E_{is} and E_{ad} were given on input cards 30 and 31 respectively.

8. END OF FILE ENCOUNTERED AFTER REFLECTION ((H(II2),II2=1,3)

9. ZERO CORLAT (M,N)

E. Next page (Final program)

Here we define SHAPE = $\exp(BOVER*\sin^2\theta/\lambda^2)$.

SCL is scale factor applied to F_{PH}. SCALE is scale factor applied to F_P.

1. Title for problem (TITLE(I),I=1,20)

2. RMS ERROR IN F IN GIVEN SIZES

(FSIZE(J,2)=1,8) number of observations in each F_{gap} range = n_{FS} where each observation is a given lack of closure for any heavy atom compound for any reflection in given range.

(FSIZE(J,1)/FSIZE(J,2),J=1,8)

$$\varepsilon^2 = \sqrt{\frac{G}{n_{FS}}} \quad \text{where } G = \sum\left(\frac{\Delta}{\text{SHAPE}}\right)^2$$

$$\text{and where } \Delta = \{\text{SCL}|F_{PH}| - |\vec{F}_P + \vec{f}_j|\}$$

$$= \{\text{SCL}|F_{PH}|_{obs} - |F_{PH}|_{calc}\}$$

i.e., r.m.s. error in F_{PH} in each range of F_{gap}

F. Next page (Final program)

1. Title for problem (TITLE(I),I=1,20)

2. For I=1,NCPDS

6. COMPOUND (I) (CPDTLE(I,1),CPDTLE(I,2))

7. MINIMUM ZONE SPACINGS FOR SHELLS Shells are $\Delta d_{GAP}, \Delta d_{GAP}/2$, etc.

(F(J),J=1,8) 1/GAP 1/2GAP etc. = minimum zone spacing

VARIATION OF CAY WITH RESOLUTION

(DAY(J),J=1,8) (CAY(I))

$$\text{DAY} = \frac{\Sigma\text{ADOBS*ADCALC*WT}}{\Sigma\text{ADCALC*ADCALC*WT}} \quad \text{vs}$$

$$\text{CAY} = \frac{\Sigma\Sigma\text{ADOBS*ADCALC*WT}}{\Sigma\Sigma\text{ADCALC*ADCALC*WT}}$$

8 terms

DERIV ES (EIS(I,J),J=1,8) $\varepsilon_{IS} = \sqrt{\frac{G}{n_\varepsilon}}$

A new set of isomorphous errors in ranges of GAP $\left(= \frac{1}{\Delta d} = \frac{\Delta d^*}{\lambda}\right)$

ANOM DISP (EAD(I,J),J=1,8) $\varepsilon_{AD} = \sqrt{\frac{G_i}{\omega}}$

$$G_1 = \sum\left(\frac{\Delta_{anom}}{\text{anom error}} * \frac{\text{SHAPE}}{\text{SCL}}\right)^2 \quad \text{where } \Delta_{anom} = |AD|_{obs} - |AD|_{calc}$$

and $|AD|_{calc} = \dfrac{2(B_P A_{HA} - A_P B_{HA})(SHAPE)}{F_{PH}}$

A new set of anomalous dispersion errors in ranges of GAP.

OLD DEL MAG NEW(SIGMA) INITIAL

3. Do for J=1,M

SCALE (OLDSCL)+(SHIFT)*(AMAGS)=(SCL)((SIGSCL))Q1(I,J) CRYSTAL NO (NZ(I,J))

BOVER (OLDB)+(DBO)*(AMAGBO)=(BOVER(I,J))((SIGBO))BOVR1(I,J)

OLD DEL MAG NEW(SIGMA) INITIAL

4. For J=1,N

ANUM (ANMOLD)+(DANUM)*(AMAGA)=(ANUM(LIST,K))((SIGDAN))ANUM1(LIST,K))

CRYSTAL NO (NZ(I,K))

X=(XOLD)+(DX)*(AMAGX)=(X(LIST))((SIGDX)) (X1(LIST))

Y=(YOLD)+(DY)*(AMAGY)=(Y(LIST))((SIGDY))(Y1(LIST))

Z=(ZOLD)+(DZ)*(AMAGZ)(Z(LIST))((SIGDZ))(Z1(LIST))

B=(BOLD(K))+(DB(K))*(AMAGB)=(B(LIST,K))((SIGDB(K))(B1(LIST,K))

NTROP(LIST) lines for B i.e., 6 if anisotropic, 1 if isotropic

i.e., K=1 to NTROP(LIST)

The standard error in the ith variable is computed from the inverted matrix as

$$\sqrt{a_{ii} \sum_{h,n} \{\omega\varepsilon^2/n-m)\}}$$

i.e., SQRT(CONST*ABS(TRIX(NV,NV)) where TRIX(NV,NV) is the appropriate diagonal term of the inverted matrix and

$$CONST = \frac{\Sigma W*EPNSQ}{(8 \text{ x } \# \text{ cpds x } \# \text{ refls} - NVAR)}$$

5. MINIMUM ZONE SPACINGS FOR SHELLS

(F(J),J=1,8) Δd $\Delta d/2$ etc.

R values in ranges of GAP.

RMS SMALL F (ECALC(M,2,J)

$$\sqrt{\frac{\Sigma FFSQ}{\Sigma 1.0}} = \sqrt{\frac{f_j^{\,2}}{N}} = \text{r.m.s. } f$$

NUM PER ZONE (ECALC(M,3,J)

$\Sigma 1.0 = n$

RMS DIFFERENCES (ECALC(M,4,J)

$$\sqrt{\frac{\Sigma(((F(MCPD)*SCL-FP)**2)}{\Sigma 1.0}} = \sqrt{\frac{(\Sigma F_{PH} - F_p)^2}{n}}$$

A.D. RESIDUALS (ECALC(M,5,J)

$$\frac{\Sigma(ADDIF)^2*WT}{\Sigma(ADCALC)^2*WT} = \frac{\Sigma(F^+ - F-)^2\ \omega}{\Sigma(AD)^2_{calc}\ \omega}$$

Require that SMALLF(f)>>ε (rms closure) for a good solution

4. STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND (M)

List for J=1,9

NUM PER ZONE (RVAL(M,1,J))

n

AVG LK OF CLOS (RVAL(M,2,J))

$$\frac{\Sigma ABS(EPS)}{\Sigma 1.0} = (\Sigma\varepsilon)/n = (\Sigma\{|F_{PHobs}|(\frac{SCL}{SHAPE})\bar{}|F_{PHcalc}|$$

AVG DERIV FPH (RVAL(M,3,J))

$$\frac{\Sigma(ABS(F(MCPD) * \frac{SHAPE}{SCL})}{\Sigma 1.0} = \frac{(\Sigma\{|F_{PH}|(\frac{SHAPE}{SCL})}{n}$$

AVG W*(E**2) (RVAL(M,4,J))

$$\frac{W*EPNSQ*10^6}{\Sigma 1.0} = \{(\Sigma\omega\varepsilon^2)/n\} \times 10^6$$

AVG W*(FPH**2) (RVAL(M,5,J))

$$\Sigma W*F(MCPD)^2*10^6 = \{(\Sigma\omega F_{PH}^{\ 2})/n\} \times 10^6$$

AVG SMALLF (RVAL(M,6,J))

$$\frac{\Sigma ABSFF}{\Sigma 1.0} = \frac{(\Sigma f_j)}{n}$$

AVG FP(NATIVE) (RVAL(M,8,J))

$$\Sigma W*(FFSQ*(\frac{SHAPE}{SCL})^2*10^6 = (\{\Sigma\omega f_j^{\,2}(\frac{SHAPE}{SCL})^2\}/n) \times 10^6$$

Small F = calculated heavy atom contribution.

5. STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND (M)

List for J=1,9

NUM PER ZONE	(RCEN(M,1,J))	as above
AVG LK OF CLOS	(RCEN(M,2,J))	as above
AVG DERIV FPH	(RCEN(M,3,J))	as above
AVG SMALL F	(RCEN(M,6,J))	as above
AVG FP(NATIVE)	(RCEN(M,7,J))	as above
AVG DELF N.C.O.	(RCEN(M,4,J))	$= \Sigma ABS(ABS(FP) - ABS(F(MCPD)*\frac{SCL}{SHAPE}))/\Sigma 1.0$
AVG DELF C.O.	(RCEN(M,5,J))	= same including terms for which A_{PH} and A_P have different signs
NUM CROSS OVERS	(RCEN(M,8,J))	= n, if A_{PH} and A_P have different signs

6. R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND (M)

List for J = 1 to 9

KRAUT R VALUE (RVAL'(M,2,J))=RVAL(M,2,J)/RVAL(M,3,J)$=\frac{\text{AVG LK OF CLOS}}{\text{AVG DERIV FPH}}$

L.S. R VALUE (RVAL'(M,4,J)=SQRT(RVAL(M,4,J)/RVAL(M,5,J))$=(\frac{\text{AVG W*(E**2)}}{\text{AVG W*(FPH**2)}})^{1/2}$

R MODULUS (RVAL'(M,6,J)=RVAL(M,2,J)/RVAL(M,6,J)$=\frac{\text{AVG LK OF CLOS}}{\text{AVG SMALLF}}$

R WEIGHTED (RVAL'(M,8,J))=RVAL(M,4,J)/RVAL(M,8,J)$=\frac{\text{AVG W*(E**2)}}{\text{AVG W*(FH**2)}}$

7. R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND (M)

List for J = 1 to 9

KRAUT R VALUE (RCEN'(M,2,J))=RCEN(M,2,J)/RCEN(M,3,J) $= \frac{\text{AVG LK OF CLOS}}{\text{AVG DERIV FPH}}$

RATIO DELF/FPH (RCEN'(M,3,J))=RCEN(M,5,J)/RCEN(M,3,J) $= \frac{\text{AVG DELF C.O.}}{\text{AVG DERIV FPH}}$

CENTRIC R VALUE (RCEN'(M,4,J))=RCEN(M,2,J)/RCEN(M,5,J) $= \frac{\text{AVG LK OF CLOS}}{\text{AVG DELF C.O.}}$

RMODULUS (RCEN'(M,6,J))=RCEN(M,2,J)/RCEN(M,6,J) $= \frac{\text{AVG LK OF CLOS}}{\text{AVG SMALLF}}$

SOD EXAMPLE (near-in reflections excluded)

COMPOUND 1

MINIMUM ZONE SPACINGS FOR SHELLS

	34.30	17.15	11.43	8.58	6.86	5.72	4.90
RMS CLOSURE	0.0	9.85	18.57	15.87	12.30	12.81	12.39
RMS EST ERROR	0.0	8.03	7.89	7.66	7.06	6.83	7.03
RMS SMALL F*	0.0	16.90	15.14	15.23	13.44	12.96	11.53
NUM PER ZONE	0.	43.	135.	250.	410.	669.	150.
RMS DIFFERENCES**	0.0	17.64	20.69	17.84	15.78	16.75	15.63
A.D. RESIDUALS	0.0	0.78	0.79	0.85	1.31	1.63	1.58

* calculated heavy atom contribution
** r.m.s. isomorphous differences

STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND 1

NUM PER ZONE	0.0	43.0	135.0	250.0	410.0	669.0	150.0
AVG LK OF CLOS	0.0	7.36	14.97	12.35	9.96	10.01	9.65
AVG DERIV FPH	0.0	60.16	49.12	44.69	47.38	51.59	51.58
AVG W*(E**2)	0.0	0.22	0.63	0.50	0.48	0.50	0.45
AVG W*(FPH**2)	0.0	10.20	5.02	5.74	8.38	9.33	9.00
AVG SMALL F	0.0	15.79	13.58	13.63	12.03	11.57	10.43
AVG FP(NATIVE)	0.0	62.98	60.46	55.11	45.26	41.52	44.05
AVG W*(FH**2)	0.0	0.78	0.45	0.62	0.58	0.51	0.39

STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND 1

NUM PER ZONE	0.0	4.0	7.0	12.0	12.0	16.0	3.0
AVG LK OF CLOS	0.0	5.44	17.69	12.14	11.08	8.75	3.45
AVG DERIV FPH	0.0	35.20	50.50	56.73	37.66	57.19	35.94
AVG SMALL F	0.0	15.61	7.75	12.12	8.58	11.98	7.37
AVG FP(NATIVE)	0.0	23.54	67.00	65.98	42.43	45.66	36.06
AVG DELF N.C.O.	0.0	11.67	17.66	15.84	10.10	13.55	9.11
AVG DELF C.O.	0.0	11.67	17.66	15.84	10.10	13.55	9.11
NUM CROSS OVERS	0.0	0.0	0.0	0.0	0.0	0.0	0.0

R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND 1

KRAUT R VALUE	0.0	0.1223	0.3047	0.2764	0.2101	0.1941	0.187
L. S. R VALUE	0.0	0.1461	0.3539	0.3235	0.3281	0.2310	0.222
R MODULUS	0.0	0.4658	1.1019	0.9058	0.8277	0.8653	0.925
R WEIGHTED	0.0	0.2784	0.3900	0.9636	0.8153	0.9706	1.131

R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND 1

KRAUT R VALUE	0.0	0.1546	0.3504	0.2139	0.2941	0.1530	0.09
RATIO DELF/FPH	0.0	0.33	0.35	0.28	0.27	0.24	0
CENTRIC R VALUE	0.0	0.4665	1.0021	0.7661	1.0968	0.6460	0.37
R MODULUS	0.0	0.3487	2.2823	1.0015	1.2901	0.7303	0.46

N.B. Usual phasing error is approximately 30° at 2 Å resolution.

Output Tapes

1. IOUT = 7 = PUNCH Formatted 3I3,1X,7F9.3

h

k

l

K_1F_p

ϕ_{best} (radians)

$K_1F_p\cos(\phi_{best})$

$K_1F_p\sin(\phi_{best})$

ϕ_{max} (radians)

$\bar{\bar{m}}$ figure of merit

2. IOUT 4 = 4 Non formatted

written if IOUT4 $\neq$ 0 and if M = MMM

h

k

l

d^*

$$\left.\begin{array}{l} SF_{PH}\cos(\phi_{best}) \\ SF_{PH}\sin(\phi_{best}) \end{array}\right\} F_{PHobs}$$

$$\left.\begin{array}{l} K_1F_p\cos(\phi_{best}) + A_{HA} \\ K_1F_p\sin(\phi_{best}) + B_{HA} \end{array}\right\} F_{PHcalc}$$

3. IOUT 3 = 3 Non formatted

h

k

l

$K_1F_p\cos(\phi_{best})$

$\bar{m}K_1F_p\cos(\phi_{best})$

$K_1F_p\sin(\phi_{best})$

$\bar{m}K_1F_p\sin(\phi_{best})$

4. IOUT 1 = 1 Non formatted

h

k

l

n_p

F_p

σF_p

AD_p

ϕ_{best}

ϕ_{max}

m

n_{PH1}

F_{PH1}

σF_{PH1}

AD_{PH1}

$\vdots$

At end IOUT 1 becomes IIN, IOUT becomes IOUT 1, IIN becomes IOUT 2

5. FOUR = 20

h

k

l

F_p

ϕ_{best} in degrees

ϕ_{max} in degrees

$$\left.\begin{array}{l} F_{PH1}\ k_2 S_1 \\ AD_{PH1}\ k_2 S_1 \\ A_{HA} \\ B_{HA} \end{array}\right\} \text{for each heavy atom}$$

$F_{PH2}\ k_2 S_2$

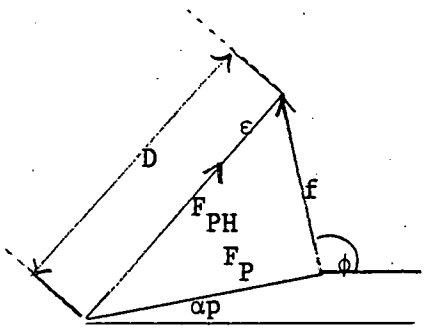
$\vdots$

k_2 = scale for heavy atom derivative = SCL

S = shape factor = exp (BOVER(I,J) $\sin^2\theta/\lambda^2$)

Theory (adapted from the writeup of Rossmann)

A. Refinement



F_{PH} = observed heavy atom derivative amplitude

D = calculated value of F_{PH}

$F_p e^{i\alpha p}$ = native protein structure factor

$fe^{i\phi}$ = heavy atom structure factor

$\varepsilon = (F_{PH} - D)$ = the "lack of closure" = the quantity to be added to F_{PH} to close the triangle

1. $D^2 = F_p^{\ 2} + f^2 + 2F_p f\cos(\alpha_p - \phi)$

$$dD = \frac{\partial D}{\partial \xi_1}\Delta\xi_1 + \frac{\partial D}{\partial \xi_2}\Delta\xi_2 \cdots$$

where $\xi_1, \xi_2 \cdots \xi_j$ are j (= number of variables) refinable parameters

2. We require that $F_{PH} = dD$, i.e., that $dD = F_{PH} - D$.

Hence we wish to minimize the quantity

$$e = \sum_h \sum_{i=1}^{N} \omega_{hi} \left[\frac{\partial D_{hi}}{\partial \xi_1}\Delta\xi_1 + \frac{\partial D_{hi}}{\partial \xi_1}\Delta\xi_2 + \cdots - (F_{PH_{hi}} - D_{hi})\right]^2$$

where there are N heavy atom derivatives (i = 1 to N)

and h independent reflections.

ω_{hi} is the weight to be applied to a given reflection for a given heavy atom derivative.

When dD is a minimum it is assumed that α_p is approximately correct.

3. Setting $\frac{\partial e}{\partial \xi_K} = 0$ for K = 1 to M we obtain the normalized equations:

$$\sum_{j=1}^{M}\left\{\sum_h \sum_{i=1}^{N} \omega_{hi} \frac{\partial D_{hi}}{\partial \xi_j}\frac{\partial D_{hi}}{\partial \xi_k}\right\}\Delta\xi_j = \sum_h \sum_{i=1}^{N} \omega_{hi} (F_{PH} - D_{hi}) \frac{\partial D_{hi}}{\partial \xi_k}$$

These equations have to be solved for the M shifts $\Delta\xi_j$.

4. We now have to consider the form of the derivative $\frac{\partial D_{hi}}{\partial \xi_i}$ for the various types of refinable parameters. It will be seen that for heavy atom derivatives i

$$D_{hi}^2 = q_i^2 \left[(a_{hi} + F_{Ph} \cos\alpha_{Ph})^2 + (b_{hi} + F_{Ph} \sin\alpha_{Ph})^2 \right]$$

where $f_{hi} = a_{hi} + ib_{hi}$ for the heavy atom structure factor of reflection h for derivative i;

F_{Ph} and α_{Ph} are the amplitude and phase of the native protein for the reflection h;

and q_i is the number by which F_{Ph} must be <u>divided</u> to bring it onto the native scale.

$$\therefore \quad \frac{\partial D}{\partial q} = \frac{D}{q}$$

and
$$\frac{\partial D}{\partial \xi} = \frac{q^2}{D} \left[(a_{hi} + F_{Ph} \cos\alpha_{Ph}) \frac{\partial a_{hi}}{\partial \xi} + (b_{hi} + F_{Ph} \sin\alpha_{Ph}) \frac{\partial b_{hi}}{\partial \xi} \right]$$

5. But since
$$a_{hi} = \sum_{n=1}^{N} Z_n \sum_{\substack{\text{equiv} \\ \text{positions}}} e^{-i\phi_s} \cos 2\pi(hx_s + ky_s + \ell z_s)$$

$$b_{hi} = \sum_{n=1}^{N} Z_n \sum_{\substack{\text{equiv} \\ \text{positions}}} e^{-i\phi_s} \sin 2\pi(hx_s + ky_s + \ell z_s)$$

and if
$$x_s = t_{11}x + t_{12}y + t_{13}z + t_{14}$$
$$y_s = t_{21}x + t_{22}y + t_{23}z + t_{24}$$
$$z_s = t_{31}x + t_{32}y + t_{33}z + t_{34}$$

then
$$\theta = 2\pi(hx_s + ky_s + \ell z_s)$$
$$= 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

where
$$h_s = t_{11}h + t_{21}k + t_{31}\ell$$
$$k_s = t_{12}h + t_{22}k + t_{32}\ell$$
$$\ell_s = t_{13}h + t_{23}k + t_{33}\ell$$
$$\Phi_s = t_{14}h + t_{24}k + t_{34}\ell$$

which gives

$$\frac{\partial a_{hi}}{\partial x} = -Z_n \sum_{equiv}^{s} 2\pi h \; e^{-i\phi_s} \sin 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

$$\frac{\partial b_{hi}}{\partial x} = -Z_n \sum_{equiv}^{s} 2\pi h \; e^{-i\phi_s} \cos 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

etc. for y and z.

6. If we have an isotropic atom

$$\phi_s = B\left(\frac{\sin\theta}{\lambda}\right)^2 \quad \text{for all values of s}$$

$$\therefore \quad \frac{\partial a_{hi}}{\partial B} = -Z_n\left(\frac{\sin\theta}{\lambda}\right)^2 \sum_{equiv}^{s} e^{-i\phi_s} \cos 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

$$\frac{\partial b_{hi}}{\partial B} = -Z_n\left(\frac{\sin\theta}{\lambda}\right)^2 \sum_{equiv}^{s} e^{-i\phi_s} \sin 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

7. If we have an anisotropic atom

$$\phi = h^2\beta_{11} + k^2\beta_{22} + \ell^2\beta_{33} + hk\beta_{12} + k\ell\beta_{23} + h\beta_{31}$$

$$\therefore \quad \phi_s = h_s^2\beta_{11} + k_s^2\beta_{22} + \ell_s^2\beta_{33} + h_s k_s\beta_{12} + k_s \ell_s\beta_{23} + \ell_s \ell_s\beta_{31}$$

and $$\frac{\partial a_{hi}}{\partial \beta_{ij}} = -Z_n \sum_{equiv}^{s} h_{si} k_{sj} \; e^{-i\phi_s} \cos 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

$$\frac{\partial b_{hi}}{\partial \beta_{ij}} = -Z_n \sum_{equiv}^{s} h_{si} k_{sj} \; e^{-i\phi_s} \sin 2\pi(h_s x + k_s y + \ell_s z + \Phi_s)$$

B. <u>Phase determination</u>

1. $\varepsilon_{hi} = F_{PHhi} - D_{hi}$. F_{PHhi} is observed, and D_{hi} is calculated for a given value of α_{Ph} as

$$D_{hi}^2 = q_i^2 \left[(a_{hi} + F_{Ph} \cos\alpha_{Ph})^2 + (b_{hi} + F_{Ph} \sin\alpha_{Ph})^2\right]$$

2. Then $P(\alpha) = \prod_{i=1}^{N} \exp\left(-\frac{\varepsilon_{hi}^2}{2E_i^2}\right)$

where ε is the "lack of closure" and E is the error in a measured F.

$P(\alpha)$ is computed at intervals $\Delta\alpha$. $\Delta\alpha$ is input to the program.

a. The most probable phase (the phase with maximum probability), i.e., α when $P(\alpha)$ has its maximum value, is fed into the least squares part of the program for the given reflection.

This phase may be used to calculate the "most probable Fourier map".

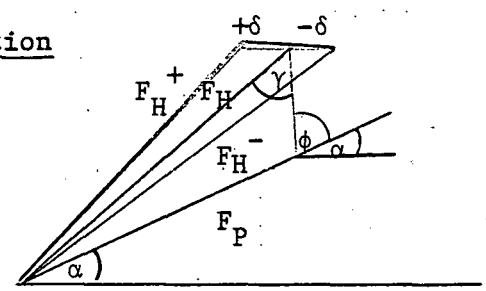
b. The best phase is used for Fourier input. The figure of merit, $\bar{m}$, is defined as

$$\bar{m} = \frac{\int_0^{2\pi} P(\alpha)\, e^{i\alpha} d\alpha}{\int_0^{2\pi} P(\alpha)\, d\alpha}$$

$$= \sqrt{\frac{(\Sigma P(\alpha)\cos\ )^2 + (\Sigma P(\alpha)\sin\alpha)^2)}{\Sigma P(\alpha)}}$$

The best phase, α_{best}, is defined as $\tan^{-1}\left(\frac{\Sigma P(\alpha)\sin\alpha}{\Sigma P(\alpha)\cos\alpha}\right)$. This is a centroid phase. In the best map these centroid phases, α_{best}, are combined with amplitudes weighted by the figure of merit. This map should have the least overall r.m.s. error in electron density.

C. <u>Anomalous dispersion as an aid to phase determination</u>



1. $F_H^{+2} = F_H^{\ 2} + \delta^2 - 2\delta F_H \cos(90-\gamma)$

$F_H^{-2} = F_H^{\ 2} + \delta^2 - 2\delta F_H \cos(90+\gamma)$

where $F_H = F_{PH}$

Therefore by subtraction

2. $F_H^{+2} - F_H^{-2} = 2\delta F_H[\cos(90+\gamma) - \cos(90-\gamma)]$

or $(F_H^+ - F_H^-) \cdot 2F_H = -4F_H \sin\gamma$

$\therefore (F_H^+ - F_H^-) = -2\sin\gamma$

3. But $\frac{\sin\gamma}{F_P} = \frac{\sin(180 + \alpha - \phi)}{F_H}$

$\therefore \quad \sin\gamma = \frac{F_P}{F_H} \sin(\phi - \alpha).$

4. By substitution

$$F_H^+ - F_H^- = \frac{2\delta F_P}{F_H} \sin(\alpha - \phi)$$

5. Let $\Delta_{OBS} = F_H^+ - F_H^-$

and $\Delta_{CALC} = \frac{2F_P\delta}{F_H} \sin(\alpha - \phi)$

Then $\varepsilon_{AD} = \Delta_{OBS} - \Delta_{CALC}$

and $P(\alpha) = \exp\left(-\frac{\varepsilon^2_{AD}}{2E^2_{AD}}\right)$

6. E^2_{AD} is the r.m.s. value of the ε_{AD} "lack of closure" for this compound over all reflections.

In calculating Δ_{CALC} for a given α the calculated value of F_H is used, not the observed value. That is

$$\Delta_{CALC} = \frac{2F_P\delta}{D} \sin(\alpha - \phi)$$

is refined in successive cycles.

7. Let $G = \frac{2F_P}{D} \sin(\alpha - \phi)$

$\therefore \quad \Delta_{CALC} = \delta G$

We wish to minimize the sum $S = \sum_h (\Delta_{OBS} - \Delta_{CALC})^2$

$$\sum_h (\Delta_{OBS} - \delta G)^2$$

$\therefore$ when $\frac{\partial S}{\partial \delta} = 0$

Then $\delta = \frac{\sum_h \Delta_{OBS} G}{\sum_h G^2}$

EXAMPLE

Input Cards

```
LEAST,STMFZ,YD1,T300.
ACCØUNT(....,...)
MØUNT(        )
ATTACH(ACCESS,ID=ZZGCPRØGS)
ACCESS(EDIT,ID=CPRØGS)
ACCESS(LEASTSQ,ID=CPRØGS)
ATTACH(DATA,....)
CØPYBF(DATA,CCD)
EDIT(INPUT,CCD,,ØUTPUT)
MØDE(0)
LDSET(PRESET=0)
LEASTSQ(,,,CCD)
EXIT.
#
J0.
M
    1    1    1    1    1    1    1

EM
000000000
 PT2 +HG EUREKA NO. 1 MAY 13 1975
  94.5    98.9       87.0                        .2                .0255
    8    2    5    3   92.     .001        25.          30.
         1.        1.        1.        1.        1.        1.        1.        1.
  1  2
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
  1  0  0 .0  0  1  0 .0  0  0  1 .0
 -1  0  0 .0  0 -1  0 .0  0  0  1 .0
  1  0  0 .0  0 -1  0 .0  0  0 -1 .0
 -1  0  0 .0  0  1  0 .0  0  0 -1 .0
  1  0  0 .5  0  1  0 .5  0  0  1 .5
 -1  0  0 .5  0 -1  0 .5  0  0  1 .5
  1  0  0 .5  0 -1  0 .5  0  0 -1 .5
 -1  0  0 .5  0  1  0 .5  0  0 -1 .5
0.
    1    1 .107     PT ANOM
 250.    250.    200.    150.    140.    130.    130.    150.
  50.    50.     50.     100.    100.    100.    100.    100.
    192.        0.
40.
    .335      .31       .21       1      11110
10.
    1    1 .107     HG ANOM
 300.    300.    200.    200.    100.    100.    100.    100.
 50.     50.     50.     50.     100.    100.    100.    100.
    1 92.5      0.
40.
    .13    .31       .31       1      11110
10.
                                                                    0

PQ
```

Card listing via Editor

```
 EDITOR.  LENGTH =  80
*EC= M
    1    1    1    1    1    1    1
OK
*EC= EM
EOF1    1758
000000000
 PT2 +HG EUREKA NO. 1 MAY 13 1975
  94.5    98.9      87.0                          .2                .0255
    8    2    5    3   92.     .001       25.          30.          1
         1.         1.         1.         1.         1.         1.         1.         1.
  1  2
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
  1  0  0 .0  0  1  0 .0  0  0  1 .0
 -1  0  0 .0  0 -1  0 .0  0  0  1 .0
  1  0  0 .0  0 -1  0 .0  0  0 -1 .0
 -1  0  0 .0  0  1  0 .0  0  0 -1 .0
  1  0  0 .5  0  1  0 .5  0  0  1 .5
 -1  0  0 .5  0 -1  0 .5  0  0  1 .5
  1  0  0 .5  0 -1  0 .5  0  0 -1 .5
 -1  0  0 .5  0  1  0 .5  0  0 -1 .5
0.
    1    1 .107      PT ANOM
 250.    250.    200.    150.    140.    130.    130.    150.
  50.     50.     50.    100.    100.    100.    100.    100.
    192.        0.
40.
    .035      .21       .21       1      11110
10.
    1    1 .107      HG ANOM
 300.    300.    200.    200.    100.    100.    100.    100.
 50.     50.     50.     50.     100.    100.    100.    100.
    1 92.5      0.
40.
    .46    .14       .48          1      11110
10.
                                                                                0
OK
*EC= PQ
EOF2    1790
*****NEW PASS*****
EDIT END.
```

Output

```
 PT2 +HG EUREKA NO. 1 MAY 13 1975
MAGNIFICATION FACTORS FOR SHIFTS ARE
FOR SCALE     1.000
FOR BOVER     1.000
FOR ANUM      1.000
FOR X,Y,Z     1.000      1.000      1.000
FOR B         1.000
RECIP=    .00011    .00010    .00013   0.00000   0.00000   0.00000
DSTMAX=   .200      DSTMIN= -0.000      GAP=       .026
NSYM=     8       NCPDS=    2       IANGLE=    5       NCYCLE=    3
SCALE= 92.000    FIGMIN=   .001    FGAP= 25.000    REJANO= 30.000    IFPRINT=    1
NPCYCL=  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
SYMMETRY CARDS
 1.00  0.00  0.00  0.00     0.00  1.00  0.00  0.00     0.00  0.00  1.00  0.00
-1.00  0.00  0.00  0.00     0.00 -1.00  0.00  0.00     0.00  0.00  1.00  0.00
 1.00  0.00  0.00  0.00     0.00 -1.00  0.00  0.00     0.00  0.00 -1.00  0.00
-1.00  0.00  0.00  0.00     0.00  1.00  0.00  0.00     0.00  0.00 -1.00  0.00
 1.00  0.00  0.00   .50     0.00  1.00  0.00   .50     0.00  0.00  1.00   .50
-1.00  0.00  0.00   .50     0.00 -1.00  0.00   .50     0.00  0.00  1.00   .50
 1.00  0.00  0.00   .50     0.00 -1.00  0.00   .50     0.00  0.00 -1.00   .50
-1.00  0.00  0.00   .50     0.00  1.00  0.00   .50     0.00  0.00 -1.00   .50
FSIZE=     0.000    -0.000    -0.000    -0.000    -0.000    -0.000    -0.000    -0.000
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND    1      PT ANOM
NATOMS =    1
NCRYST =    1
CAY =     .1070
EIS=   250.000   250.000   200.000   150.000   140.000   130.000   130.000   150.000
CAD=    50.000    50.000    50.000   100.000   100.000   100.000   100.000   100.000
CRYSTAL NO.  1  NZ(I,J)=  1
SCALE =   92.0000
BOVER =    0.0000  IFBOVR =-0
ANUMS =   40.0000
COORDINATES =  .0350  .2100  .2100
```

```
NTROP= 1   B =    10.000    -0.000    -0.000    -0.000    -0.000    -0.000
LABEL =  1  1  1  1  0
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND   2     HG ANOM
NATOMS =    1
NCRYST =    1
CAY =     .1070
EIS=   300.000   300.000   200.000   200.000   100.000   100.000   100.000   100.000
EAD=    50.000    50.000    50.000    50.000   100.000   100.000   100.000   100.000
CRYSTAL NO.  1  NZ(I,J)=  1
SCALE =   92.5000
BOVER =    0.0000  IFBOVR =-0
ANUMS =   40.0000
COORDINATES =  .4600  .1400  .4800
NTROP= 1   B =    10.000    -0.000    -0.000    -0.000    -0.000    -0.000
LABEL =  1  1  1  1  0
END OF FILE ENCOUNTERED AFTER REFLECTION  18.  6.  0.
ZERO CORLAT   11    1
 PT2 +HG EUREKA NO. 1 MAY 13 1975
CORRELATION MATRIX
    1.0000    -.0612     .0329     .0090    -.0154    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    1.0000     .0359    -.0025     .0558    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    1.0000    -.0058     .0075    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    1.0000    -.0174    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    0.0000    1.0000    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.1482     .0182     .0053     .0490
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0039     .0300    -.1068
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0101    -.0470
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0057
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000
 PT2 +HG EUREKA NO. 1 MAY 13 1975
RMS ERROR IN F IN GIVEN SIZES
       0.0       0.0       0.0       0.0       0.0       0.0       0.0    2716.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0     124.1
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 1     PT ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22    19.61    13.07     9.80     7.84     6.54     5.60     4.90
VARIATION OF CAY WITH RESOLUTION
               0.00000   .05320   .15587   .01787   .02408   .07831   .08381   .07691        .06766
DERIV  ES          0.0    252.4    153.2    123.1    128.5    122.5    109.6    147.7
ANOM DISP          0.0     39.4     71.5     87.5    106.0    104.1     91.9    112.4
          OLD      DEL     MAG        NEW( SIGMA)   INITIAL
SCALE 92.0000 + 5.0656 * 1.00 =  97.0656( .0000)   92.0000   CRYST NO  1
BOVER    0.00 +   0.00 * 1.00 =    0.00( 0.00)      0.00
          OLD      DEL     MAG        NEW( SIGMA)   INITIAL
ANUM     40.00 +   3.48 * 1.00 =   43.48( 1.29)     40.00   CRYST NO  1
  X      .0350 + -.0014 * 1.00 =   .0336( .0005)     .0350
  Y      .2100 +  .0005 * 1.00 =   .2105( .0006)     .2100
  Z      .2100 + -.0010 * 1.00 =   .2090( .0007)     .2100
  B      10.00 +   0.00 * 1.00 =   10.00( 0.00)      10.00
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 2     HG ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22    19.61    13.07     9.80     7.84     6.54     5.60     4.90
VARIATION OF CAY WITH RESOLUTION
               0.00000   .13972   .10599   .21292   .07248   .07920   .05553   .06510        .08494
DERIV  ES          0.0    363.5    151.4    129.6     95.3     88.8     95.9    102.5
ANOM DISP          0.0     41.3     56.6     68.6     94.9     99.3    114.1    122.3
          OLD      DEL     MAG        NEW( SIGMA)   INITIAL
SCALE 92.5000 +  .5456 * 1.00 =  93.0456( .0000)   92.5000   CRYST NO  1
 OVER    0.00 +   0.00 * 1.00 =    0.00( 0.00)      0.00
          OLD      DEL     MAG        NEW( SIGMA)   INITIAL
```

```
ANUM      40.00 +   1.10 * 1.00 =    41.10(  1.12)      40.00   CRYST NO  1
  X       .4600 + -.0001 * 1.00 =    .4599( .0004)      .4600
  Y       .1400 + -.0001 * 1.00 =    .1399( .0004)      .1400
  Z       .4800 + -.0015 * 1.00 =    .4785( .0005)      .4800
  B       10.00 +   0.00 * 1.00 =    10.00(  0.00)      10.00
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
R MODULUS        0.0000  1.3402   .8910   .7463   .5400   .4957   .5101   .6342        .6007
R WEIGHTED       0.0000  2.8229  1.0263   .7479   .5000   .4284   .4487   .7007        .5482
FIG MERIT        0.0000   .4692   .3871   .4209   .4791   .4617   .4317   .4346        .4430
                    0.     24.     75.    135.    222.    302.    344.    383.         1485.
FIGURE OF MERIT DISTRIBUTION
      130.      180.      185.      194.      178.      190.      170.      128.      50.      80.
       .05       .15       .25       .35       .45       .55       .65       .75       .85      .95
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 1      PT ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
RMS CLOSURE        0.00  252.42  153.24  123.11  128.49  122.50  109.60  147.67
RMS EST. ERROR     0.00  204.48  273.87  340.43  301.05  395.48  406.27  474.74
RMS SMALLF         0.00  160.18  154.47  149.16  156.45  153.25  150.48  145.70
NUM PER ZONE       0.     23.     73.    131.    214.    291.    339.    380.
RMS DIFFERENCES    0.00  299.27  223.13  190.03  180.95  162.49  140.14  185.34
A.D.RESIDUALS      0.00    1.59    2.91    3.38    3.66    3.98    3.70    4.47
STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND      1
NUM PER ZONE       0.0     23.0    73.0   131.0   214.0   291.0   339.0   380.0       1451.0
AVG LK OF CLOS     0.00  201.47  113.94   90.29   89.71   80.19   73.76   94.72        88.43
AVG DERIV FPH      0.00  695.28  689.68  736.96  733.09  711.86  758.74  819.38       754.99
AVG W*(E**2)       0.00    1.02     .59     .67     .84     .89     .71     .97          .83
AVG W*(FPH**2)     0.00    8.16   12.50   25.47   28.64   30.79   34.92   30.65        29.64
AVG SMALL F        0.00  152.54  134.10  129.80  139.43  137.98  135.09  131.11       135.02
AVG FP(NATIVE)     0.00  541.32  685.29  811.10  816.09  732.25  744.44  836.47       776.49
AVG W*(FH**2)      0.00     .41     .60     .99    1.25    1.39    1.34     .94         1.15
STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND      1
NUM PER ZONE       0.0     12.0    24.0    36.0    45.0    51.0    57.0    54.0        279.0
AVG LK OF CLOS     0.00  253.37  169.53  116.37  136.35  157.14  131.68  165.42       150.13
AVG DERIV FPH      0.00  678.81  627.13  685.99  744.06  701.13  734.95  785.22       721.96
AVG SMALL F        0.00  154.85   92.63   88.00  115.11  125.55  146.32  134.16       123.36
AVG FP(NATIVE)     0.00  531.61  691.49  762.81  899.33  810.45  769.94  936.63       812.56
AVG DELF N.C.O.    0.00  302.83  212.48  150.73  183.12  174.69   89.97  201.05       169.51
AVG DELF C.O.      0.00  302.83  212.48  150.73  183.12  174.69   89.97  201.05       169.51
NUM CROSS OVERS    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00         0.00
R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND        1
KRAUT R VALUE    0.0000   .2898   .1652   .1225   .1224   .1126   .0972   .1156        .1171
L. S. R VALUE    0.0000   .3535   .2167   .1626   .1715   .1698   .1427   .1778        .1672
R MODULUS        0.0000  1.3208   .8497   .6956   .6434   .5812   .5460   .7225        .6549
R WEIGHTED       0.0000  2.4834   .9840   .6812   .6745   .6389   .5305  1.0272        .7213
R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND        1
KRAUT R VALUE    0.0000   .3733   .2703   .1696   .1833   .2241   .1792   .2107        .2080
RATIO DELF/FPH     0.00     .45     .34     .22     .25     .25     .12     .26          .23
CENTRIC R VALUE  0.0000   .8367   .7979   .7721   .7445   .8995  1.4637   .8227        .8857
R MODULUS        0.0000  1.6362  1.8303  1.3224  1.1846  1.2517   .8999  1.2330       1.2170
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 2      HG ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
RMS CLOSURE        0.00  363.53  151.44  129.59   95.33   88.83   95.88  102.48
RMS EST. ERROR     0.00  175.21  232.04  289.79  318.13  321.79  354.94  417.59
RMS SMALLF         0.00  205.36  146.11  137.76  150.40  161.73  153.61  143.06
NUM PER ZONE       0.     22.     72.    133.    210.    257.    266.    305.
RMS DIFFERENCES    0.00  458.60  196.90  159.63  132.00  131.57  140.22  147.38
A.D.RESIDUALS      0.00    2.35    2.49    3.33    3.71    3.58    3.92    4.75
STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND      2
```

```
NUM PER ZONE          0.0     22.0     72.0    133.0    210.0    257.0    266.0    305.0     1265.0
AVG LK OF CLOS       0.00   256.34   120.71    98.47    59.26    58.17    61.86    66.32      72.34
AVG DERIV FPH        0.00   847.26   810.54   875.82   855.73   764.49   734.67   820.23     802.57
AVG W*(E**2)         0.00     1.47      .57      .42      .91      .79      .92     1.05        .86
AVG W*(FPH**2)       0.00     8.96    18.62    21.76    81.77    62.91    57.10    72.90      50.44
AVG SMALL F          0.00   188.95   129.18   123.26   136.93   144.30   133.39   127.33     134.39
AVG FP(NATIVE)       0.00   526.45   686.23   802.87   817.47   743.15   765.62   866.69     789.27
AVG W*(FH**2)        0.00      .47      .53      .47     2.26     2.62     2.36     2.05       1.99
STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND        2
NUM PER ZONE         0.0     11.0     23.0     39.0     39.0     47.0     44.0     44.0      247.0
AVG LK OF CLOS       0.00   309.37   133.79   129.33   133.48   125.80   107.67   143.18     136.36
AVG DERIV FPH        0.00   835.70   740.44   811.77   949.50   823.19   769.68   994.56     855.18
AVG SMALL F          0.00   212.42   120.21   123.44   121.34   134.35    98.51    96.94     119.69
AVG FP(NATIVE)       0.00   500.98   594.72   731.97   937.76   820.44   788.84  1003.53     826.05
AVG DELF N.C.O.      0.00   398.22   117.71   142.74   131.29   123.66   125.37   149.40     144.44
AVG DELF C.O.        0.00   398.22   117.71   142.74   131.29   123.66   125.37   149.40     144.44
NUM CROSS OVERS      0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00       0.00
R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND        2
KRAUT R VALUE      0.0000    .3026    .1483    .1124    .0692    .0761    .0842    .0809      .0901
L. S. R VALUE      0.0000    .4048    .1755    .1389    .1054    .1120    .1269    .1200      .1203
R MODULUS          0.0000   1.3587    .9345    .7969    .4327    .4031    .4638    .5209      .5382
R WEIGHTED         0.0000   3.1338   1.0742    .8849    .4018    .3017    .3895    .5131      .4332
R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND        2
KRAUT R VALUE      0.0000    .3702    .1807    .1593    .1406    .1528    .1399    .1440      .1594
RATIO DELF/FPH       0.00      .48      .16      .18      .14      .15      .16      .15        .17
CENTRIC R VALUE    0.0000    .7769   1.1366    .9060   1.0167   1.0173    .8588    .9584      .9440
R MODULUS          0.0000   1.4564   1.1139   1.0477   1.1001    .9363   1.0931   1.4770     1.1393

END OF FILE ENCOUNTERED AFTER REFLECTION  18.  6.  0.
ZERO CORLAT   11    1
 PT2 +HG EUREKA NO. 1 MAY 13 1975
CORRELATION MATRIX
    1.0000    -.2230     .0390     .0160    -.0026    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    1.0000     .0268    -.0100     .0491    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    1.0000    -.0088     .0137    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    1.0000    -.0112    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    0.0000    1.0000    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.2328     .0111    -.0004     .0267
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000     .0108     .0122    -.0939
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0033    -.0367
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0101
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000
 PT2 +HG EUREKA NO. 1 MAY 13 1975
RMS ERROR IN F IN GIVEN SIZES
      -0.0       0.0       0.0       0.0       0.0       0.0       0.0    2716.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0     121.1
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 1      PT ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22     19.61     13.07      9.80      7.84      6.54      5.60      4.90
VARIATION OF CAY WITH RESOLUTION
               0.00000    .04643   .07076  -.02858    .00675    .06736    .06285    .07285     .04367
DERIV ES           0.0     248.8     148.1     118.1     119.8     123.0     110.7     136.0
ANOM DISP          0.0      39.3      81.6      92.9     110.9     110.1      97.8     118.6
            OLD       DEL     MAG        NEW( SIGMA)   INITIAL
SCALE   97.0656 + 2.3384 * 1.00 =  99.4040( .0000)   92.0000   CRYST NO  1
BOVER     0.00 +    0.00 * 1.00 =    0.00( 0.00)      0.00
            OLD       DEL     MAG        NEW( SIGMA)   INITIAL
ANUM     43.48 +    3.00 * 1.00 =   46.48( 1.19)     40.00   CRYST NO  1
  X      .0336 + -.0012 * 1.00 =    .0324( .0005)     .0350
  Y      .2105 +  .0006 * 1.00 =    .2111( .0005)     .2100
  Z      .2090 + -.0004 * 1.00 =    .2086( .0006)     .2100
  B      10.00 +    0.00 * 1.00 =   10.00( 0.00)     10.00
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 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 2      HG ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                    39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
VARIATION OF CAY WITH RESOLUTION
                  0.00000  .13241  .09346  .08452  .04914  .05152  .04670  .04670        .05613
DERIV  ES           0.0    391.8   150.2   112.6    95.2    87.3    98.2   102.6
ANOM DISP           0.0     41.7    57.8    75.8    36.3   101.2   114.8   123.4
            OLD      DEL     MAG        NEW( SIGMA)   INITIAL
SCALE  93.0456 +   .1440 * 1.00 =  93.1896( .0000)   92.5000   CRYST NO  1
BOVER     0.00 +    0.00 * 1.00 =    0.00( 0.00)      0.00
            OLD      DEL     MAG        NEW( SIGMA)   INITIAL
ANUM     41.10 +   1.17 * 1.00 =    42.27( 1.24)     40.00   CRYST NO  1
  X      .4599 + -.0001 * 1.00 =    .4598( .0005)    .4600
  Y      .1399 + -.0003 * 1.00 =    .1396( .0005)    .1400
  Z      .4785 + -.0017 * 1.00 =    .4769( .0006)    .4803
  B      10.00 +   0.00 * 1.00 =   10.00( 0.00)     10.00
MINIMUM ZONE SPACINGS FOR SHELLS
                    39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
R MODULUS          0.0000  1.3141   .8293   .6284   .4848   .4668   .4967   .5876         .5571
R WEIGHTED         0.0000  2.6362   .8804   .5727   .4352   .4022   .4304   .6147         .5080
FIG MERIT          0.0000   .4399   .5236   .5355   .4995   .5128   .5087   .4669         .4995
                      0.     24.     75.    135.    222.    302.    344.    383.         1485.
FIGURE OF MERIT DISTRIBUTION
      98.      123.      146.      174.      183.      201.      203.      170.      92.      95.
      .05      .15       .25       .35       .45       .55       .65       .75       .85      .95
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 1      PT ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                    39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
 MS CLOSURE         0.00  248.83  148.05  118.08  119.78  122.97  110.66  135.97
 MS EST. ERROR      0.00  212.95  283.43  351.87  394.35  410.02  419.91  490.69
RMS SMALLF          0.00  175.65  168.31  162.50  169.42  165.91  163.31  159.12
NUM PER ZONE        0.     23.     73.    131.    214.    291.    339.    380.
RMS DIFFERENCES     0.00  326.25  225.44  173.61  162.93  162.58  152.35  189.03
A.D.RESIDUALS       0.00    2.46    4.80    5.14    5.68    6.32    6.02    7.47
STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND      1
NUM PER ZONE        0.0    23.0    73.0   131.0   214.0   291.0   339.0   380.0        1451.0
AVG LK OF CLOS      0.00  194.83  112.29   83.99   82.02   80.80   74.97   92.10         86.26
AVG DERIV FPH       0.00  733.56  727.66  777.53  773.45  751.06  800.52  864.49        796.56
AVG W*(E**2)        0.00     .78     .56     .46     .45     .50     .45     .50           .48
AVG W*(FPH**2)      0.00    7.17   14.32   20.88   19.59   19.05   23.98   20.63         20.44
AVG SMALL F         0.00  167.03  147.04  141.45  150.84  149.35  147.23  143.48        146.99
AVG FP(NATIVE)      0.00  541.32  685.29  811.10  816.09  732.25  744.44  836.47        776.49
AVG W*(FH**2)       0.00     .39     .73     .86     .90     .91     .97     .68           .84
STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND      1
NUM PER ZONE        0.0    12.0    24.0    36.0    45.0    51.0    57.0    54.0         279.0
AVG LK OF CLOS      0.00  233.84  161.86  119.87  134.19  155.49  133.86  152.21        146.33
AVG DERIV FPH       0.00  716.18  661.66  723.76  785.02  739.74  775.42  828.46        761.71
AVG SMALL F         0.00  172.12  100.23   96.29  121.72  130.95  157.74  152.08        134.20
AVG FP(NATIVE)      0.00  531.61  691.49  762.81  899.33  810.45  769.94  936.63        812.56
AVG DELF N.C.O.     0.00  325.52  209.63  141.53  161.30  164.06   98.20  183.30        161.84
AVG DELF C.O.       0.00  325.52  209.63  141.53  161.30  164.06   98.20  183.30        161.84
NUM CROSS OVERS     0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00          0.00
R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND        1
KRAUT R VALUE      0.0000   .2656   .1543   .1080   .1060   .1076   .0937   .1065         .1083
L. S. R VALUE      0.0000   .3303   .1984   .1478   .1515   .1616   .1365   .1552         .1537
R MODULUS          0.0000  1.1665   .7637   .5938   .5438   .5410   .5092   .6419         .5868
R WEIGHTED         0.0000  2.0069   .7738   .5280   .4999   .5493   .4591   .7303         .5740
R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND        1
KRAUT R VALUE      0.0000   .3265   .2446   .1656   .1709   .2102   .1726   .1837         .1921
RATIO DELF/FPH      0.00     .45     .32     .20     .21     .22     .13     .22           .21
CENTRIC R VALUE    0.0000   .7184   .7721   .8470   .8320   .9478  1.3632   .8304         .9041
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R MODULUS	0.0000	1.3586	1.5237	1.2450	1.1025	1.1874	.8486	1.0009	1.0904

PT2 +HG EUREKA NO. 1 MAY 13 1975

COMPOUND 2 HG ANOM

MINIMUM ZONE SPACINGS FOR SHELLS

	39.22	19.61	13.07	9.80	7.84	6.54	5.60	4.90	
RMS CLOSURE	0.00	391.75	150.20	112.58	95.19	87.31	98.15	102.60	
RMS EST. ERROR	0.00	175.91	232.69	290.58	319.00	322.72	355.93	418.74	
RMS SMALLF	0.00	209.42	148.97	141.38	155.42	166.38	156.26	145.80	
NUM PER ZONE	0.	22.	72.	133.	210.	257.	266.	305.	
RMS DIFFERENCES	0.00	463.23	200.27	162.62	134.18	132.82	139.86	146.67	
A.D.RESIDUALS	0.00	2.72	3.15	4.36	4.53	4.40	4.84	5.85	
STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND					2				
NUM PER ZONE	0.0	22.0	72.0	133.0	210.0	257.0	266.0	305.0	1265.0
AVG LK OF CLOS	0.00	279.19	119.49	84.50	59.24	56.59	64.90	66.45	71.54
AVG DERIV FPH	0.00	852.26	815.33	880.98	860.78	769.00	739.01	825.07	807.31
AVG W*(E**2)	0.00	1.04	.59	.39	.37	.33	.39	.41	.40
AVG W*(FPH**2)	0.00	51.53	19.66	27.37	33.80	27.34	23.50	28.49	27.07
AVG SMALL F	0.00	192.85	132.30	126.80	140.86	148.09	135.42	129.60	137.41
AVG FP(NATIVE)	0.00	526.45	686.23	802.87	817.47	743.15	765.62	866.69	789.27
AVG W*(FH**2)	0.00	.30	.58	.62	.99	1.19	.99	.82	.92
STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND					2				
NUM PER ZONE	0.0	11.0	23.0	39.0	39.0	47.0	44.0	44.0	247.0
AVG LK OF CLOS	0.00	343.29	133.92	114.16	132.15	121.55	106.91	146.07	134.84
AVG DERIV FPH	0.00	840.63	744.81	816.56	955.10	828.05	774.22	1000.43	860.22
AVG SMALL F	0.00	215.92	121.06	122.71	119.45	133.85	98.61	98.11	119.64
AVG FP(NATIVE)	0.00	500.98	694.72	731.97	937.76	820.44	788.84	1003.53	826.05
AVG DELF N.C.O.	0.00	401.81	119.19	145.27	132.72	125.54	125.85	150.38	145.98
AVG DELF C.O.	0.00	401.81	119.19	145.27	132.72	125.54	125.85	150.38	145.98
NUM CROSS OVERS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND					2				
KRAUT R VALUE	0.0000	.3276	.1465	.0959	.0688	.0736	.0878	.0805	.0886
L. S. R VALUE	0.0000	.4337	.1730	.1200	.1046	.1094	.1201	.1195	.1218
R MODULUS	0.0000	1.4477	.9032	.6664	.4205	.3821	.4792	.5127	.5206
R WEIGHTED	0.0000	3.4995	1.0166	.6340	.3751	.2754	.3946	.4952	.4384
R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND					2				
KRAUT R VALUE	0.0000	.4084	.1798	.1398	.1384	.1468	.1381	.1460	.1568
RATIO DELF/FPH	0.00	.48	.16	.18	.14	.15	.16	.15	.17
CENTRIC R VALUE	0.0000	.8544	1.1236	.7859	.9957	.9683	.8495	.9713	.9237
R MODULUS	0.0000	1.5899	1.1062	.9303	1.1063	.9081	1.0841	1.4889	1.1271

Reflection data

0	0	4	341.32	6.283	6.283	.29	1	0.00	0.00	0.00	360	0.0	0.0	2	503.22	0.00	279.69	360	279.7	-1.2
0	0	8	602.60	6.283	6.283	.99	1	373.76	0.00	180.68	540	-180.7	.8	2	652.33	0.00	130.68	360	130.7	-.6
0	0	10	1651.40	3.142	3.142	.95	1	1503.98	0.00	307.57	360	307.6	-1.3	2	2060.42	0.00	35.60	360	35.6	-.2
0	1	3	420.44	3.142	3.142	.66	1	668.00	0.00	63.14	540	-63.1	.3	2	845.23	0.00	193.93	540	-193.9	.9
0	1	5	762.68	3.142	3.142	.96	1	438.37	0.00	86.05	360	86.0	-.4	2	857.34	0.00	160.80	540	-160.8	.7
0	1	7	1104.00	6.283	6.283	.95	1	797.22	0.00	85.58	540	-85.6	.4	2	1049.32	0.00	110.93	540	-110.9	.5
0	1	17	779.24	6.283	6.283	.27	1	611.33	0.00	78.49	540	-78.5	.3	2	750.18	0.00	155.13	360	155.1	-.7
0	2	6	436.08	6.283	6.283	.05	1	0.00	0.00	0.00	540	0.0	0.0	2	406.31	0.00	38.91	540	-38.9	.2
0	2	8	780.16	3.142	3.142	.75	1	725.65	0.00	159.35	360	159.4	-.7	2	1113.62	0.00	23.31	540	-23.3	.1
0	2	10	581.44	3.254	3.142	.00	1	0.00	0.00	0.00	360	0.0	0.0	2	581.50	0.00	7.00	540	-7.0	.0

0. 2. 10. F NATIVE= 581. FIG OF MERIT= .000 BEST AND MOST PROBABLE PHASES ARE 186, 180.

CPD	FH	AD	FSMALL	PHI	A	B
1	0.	0.	0.	360	0.	0.
2	582.	0.	7.	540	-7.	.0.

TOTAL PHASE PROBABILITY CURVE

1.00 1.00

1.00 1.00

0	2	14	1322.96	6.283	6.283	.98	1	913.52	0.00	269.53	540	-269.5	1.2	2	1491.03	0.00	26.42	360	26.4	-.1
0	3	3	448.04	6.283	6.283	.31	1	524.85	0.00	174.32	360	174.3	-.8	2	506.95	0.00	264.81	360	264.8	-1.2
0	3	5	1536.40	6.283	6.283	.98	1	1075.55	0.00	237.54	540	-237.5	1.0	2	1597.27	0.00	218.34	360	218.3	-1.0
0	3	7	399.28	6.283	6.283	1.00	1	571.57	0.00	236.20	360	236.2	-1.0	2	800.50	0.00	150.62	360	150.6	-.7
0	3	9	1417.72	6.283	6.283	.98	1	1092.45	0.00	171.44	540	-171.4	.8	2	1464.94	0.00	72.77	360	72.8	-.3
0	3	11	966.92	3.142	3.142	.74	1	785.29	0.00	66.73	360	66.7	-.3	2	1100.57	0.00	8.68	540	-8.7	.0
17	6	5	1363.44	4.408	3.054	.20	1	849.90	-15.90	41.78	401	31.7	27.2	2	1404.37	-49.39	165.92	253	-48.9	-158.5
17	7	0	1054.32	3.142	3.142	1.00	1	843.94	0.00	317.85	360	317.8	-1.4	2	751.11	0.00	125.26	360	125.3	-.6
17	7	2	989.92	6.192	5.149	.41	1	883.70	19.88	275.02	538	-274.9	8.9	2	999.92	-22.37	118.14	365	117.7	10.6
17	7	4	771.88	5.852	5.061	.34	1	946.33	-122.27	161.44	355	160.9	-13.6	2	720.36	165.88	104.14	372	102.0	21.1
17	8	1	907.12	4.135	4.101	.29	1	1024.86	0.00	100.68	288	30.9	-95.8	2	964.51	43.80	94.95	523	-90.7	20.2
18	0	0	1092.96	6.283	6.283	.79	1	800.20	0.00	296.31	540	-296.3	1.3	2	1341.93	0.00	49.64	540	-49.6	.2
18	0	2	954.96	3.142	3.142	.36	1	882.71	0.00	256.28	360	256.3	-1.1	2	825.66	0.00	50.08	540	-50.1	.2
18	0	4	650.44	3.142	3.142	.99	1	871.77	0.00	147.38	540	-147.4	.7	2	895.55	0.00	43.38	540	-43.4	.2
18	1	1	800.40	2.134	2.792	.34	1	854.87	199.80	159.21	456	-17.2	158.3	2	694.26	20.50	46.55	313	31.9	-33.9
18	1	3	752.56	1.739	.785	.31	1	823.07	-162.03	126.78	293	50.1	-116.5	2	623.44	-180.79	102.51	286	28.4	-98.5
18	1	5	1442.56	4.869	4.887	.75	1	930.42	13.92	80.49	507	-67.9	43.3	2	1740.78	-31.68	156.51	279	24.1	-154.6
18	2	0	930.12	3.142	3.142	.53	1	882.71	0.00	261.27	360	261.3	-1.1	2	1023.22	0.00	9.52	360	9.5	-.0
18	2	2	1177.60	.122	.262	.76	1	934.40	40.76	228.64	530	-225.1	39.8	2	1258.06	-48.46	85.38	444	9.0	84.9
18	2	4	1376.32	3.206	3.142	.70	1	991.06	42.74	147.31	332	130.3	-68.7	2	1300.00	-51.25	164.57	447	8.2	164.4
18	3	1	895.16	.297	.349	.31	1	912.53	90.46	130.90	292	49.5	-121.2	2	766.02	-18.64	48.79	206	-43.9	-21.3
18	3	3	735.08	3.284	3.403	.71	1	949.31	-122.27	164.13	507	-137.8	89.1	2	916.05	13.05	73.43	238	-39.4	-62.0
18	4	0	757.16	3.142	3.142	.90	1	889.67	0.00	164.85	540	-164.8	.7	2	684.94	0.00	46.14	360	46.1	-.2
18	4	2	813.28	5.932	.873	.20	1	902.59	-62.62	157.81	334	141.7	-69.4	2	775.34	49.39	55.21	325	45.2	-31.7
18	5	1	853.76	5.425	5.236	.26	1	772.37	221.67	88.23	501	-68.6	55.5	2	807.02	-103.44	44.16	471	-15.7	41.3
18	6	0	608.12	6.283	6.283	.48	1	976.15	0.00	31.71	360	31.7	-.1	2	646.74	0.00	27.08	540	-27.1	.1

END OF FILE ENCOUNTERED AFTER REFLECTION 18. 6. 0.

```
ZERO CORLAT    11     1
 PT2 +HG EUREKA NO. 1 MAY 13 1975
CORRELATION MATRIX
    1.0000    -.2956     .0500     .0362     .0049    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    1.0000     .0171    -.0129     .0364    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    1.0000    -.0039     .0091    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    1.0000    -.0044    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    0.0000    1.0000    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.2670    -.0001     .0017     .0322
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000     .0277     .0148    -.0660
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0035    -.0280
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000    -.0097
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    1.0000
 PT2 +HG EUREKA NO. 1 MAY 13 1975
RMS ERROR IN F IN GIVEN SIZES
       0.0       0.0       0.0       0.0       0.0       0.0       0.0    2716.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0     120.5
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 1      PT ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22    19.61    13.07     9.80     7.84     6.54     5.60     4.90
  IRIATION OF CAY WITH RESOLUTION
      ζ          0.00000   .04946   .06084 -.03974 -.00331   .05702   .03180   .06372        .02863
DERIV  ES           0.0    223.9    146.4    110.0    116.9    120.7    111.9    131.9
ANOM DISP           0.0     39.6     84.0     94.1    113.1    113.1    101.1    121.9
            OLD      DEL     MAG        NEW( SIGMA)   INITIAL
SCALE   99.4040 + 1.1505 * 1.00 = 100.5546( .0000)   92.0000   CRYST NO  1
COVER      0.00 +   0.00 * 1.00 =     0.00( 0.00)      0.00
            OLD      DEL     MAG        NEW( SIGMA)   INITIAL
ANUM      46.48 +   2.44 * 1.00 =    48.93( 1.19)     40.00   CRYST NO  1
  X       .0324 + -.0010 * 1.00 =    .0314( .0004)    .0350
  Y       .2111 +  .0005 * 1.00 =    .2116( .0005)    .2100
  Z       .2036 + -.0000 * 1.00 =    .2086( .0005)    .2100
  B       10.00 +   0.00 * 1.00 =    10.00( 0.00)     10.00
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 2      HG ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                 39.22    19.61    13.07     9.80     7.84     6.54     5.60     4.90
VARIATION OF CAY WITH RESOLUTION
                 0.00000   .08614   .08916   .06081   .03529   .03406   .00233   .01403        .03203
DERIV  ES           0.0    430.6    149.7    114.8     87.9     91.0     99.7    103.4
ANOM DISP           0.0     44.4     58.5     76.7     96.5    101.7    116.1    124.2
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```
            OLD       DEL     MAG          NEW( SIGMA)    INITIAL
SCALE  93.1896 +   .2671 * 1.00 =  93.4568( .0000)   92.5000    CRYST NO  1
BOVER      0.00 +    0.00 * 1.00 =      0.00(  0.00)      0.00
            OLD       DEL     MAG          NEW( SIGMA)    INITIAL
ANUM     42.27 +     .49 * 1.00 =    42.77(  1.26)     40.00    CRYST NO  1
  X      .4598 + -.0001 * 1.00 =    .4597( .0004)     .4600
  Y      .1396 + -.0000 * 1.00 =    .1396( .0005)     .1400
  Z      .4769 + -.0021 * 1.00 =    .4748( .0006)     .4800
  B      10.00 +   0.00 * 1.00 =    10.00(  0.00)     10.00
MINIMUM ZONE SPACINGS FOR SHELLS
                    39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
R MODULUS          0.0000  1.2835   .7833   .5040   .4498   .4471   .4786   .5571        .5289
R WEIGHTED         0.0000  2.3559   .7864   .4955   .3606   .3703   .4042   .5462        .4552
FIG MERIT          0.0000   .4507   .5435   .5662   .5189   .5292   .5264   .5103        .5250
                       0.     24.     75.    135.    222.    302.    344.    383.        1485.
FIGURE OF MERIT DISTRIBUTION
      87.      102.      133.      154.      184.      198.      219.      190.      106.      104.
     .05       .15       .25       .35       .45       .55       .65       .75       .85       .95
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 1     PT ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                    39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
RMS CLOSURE         0.00  223.92  146.36  110.04  116.95  120.74  111.06  131.91
RMS EST. ERROR      0.00  216.90  287.90  357.23  400.57  416.81  426.30  498.15
RMS SMALLF          0.00  189.13  180.36  173.95  180.43  176.70  174.26  170.61
NUM PER ZONE        0.     23.     73.    131.    214.    291.    339.    380.
RMS DIFFERENCES     0.00  339.52  228.74  168.99  157.59  165.86  161.46  194.38
A.D.RESIDUALS       0.00    3.68    7.13    7.48    8.37    9.52    9.25   11.68
STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND      1
NUM PER ZONE         0.0    23.0    73.0   131.0   214.0   291.0   339.0   380.0       1451.0
AVG LK OF CLOS      0.00  176.56  111.81   80.01   78.89   80.53   75.77   90.38        84.80
AVG DERIV FPH       0.00  751.24  745.19  796.26  792.09  769.15  819.80  885.32       815.75
AVG W*(E**2)        0.00     .65     .59     .42     .47     .49     .47     .52          .49
AVG W*(FPH**2)      0.00    7.77   15.96   23.39   22.59   20.39   25.61   24.28        22.80
AVG SMALL F         0.00  179.38  158.59  151.35  160.09  158.83  158.09  154.06       157.23
AVG FP(NATIVE)      0.00  541.32  685.29  811.10  816.09  732.25  744.44  836.47       776.49
AVG W*(FH**2)       0.00     .47     .89    1.06    1.12    1.05    1.13     .88         1.02
STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND      1
NUM PER ZONE         0.0    12.0    24.0    36.0    45.0    51.0    57.0    54.0        279.0
AVG LK OF CLOS      0.00  200.58  157.77  108.61  135.56  147.11  135.09  145.59       140.75
AVG DERIV FPH       0.00  733.44  677.60  741.20  803.94  757.56  794.10  848.41       780.06
AVG SMALL F         0.00  187.21  119.69  102.52  126.40  133.82  165.80  166.68       142.56
AVG FP(NATIVE)      0.00  531.61  691.49  762.81  899.33  810.45  769.94  936.63       812.56
AVG DELF N.C.O.     0.00  335.99  208.35  137.45  152.65  160.20  106.07  176.63       159.87
AVG DELF C.O.       0.00  335.99  208.35  137.45  152.65  160.20  106.07  176.63       159.87
NUM CROSS OVERS     0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00         0.00
R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND        1
KRAUT R VALUE     0.0000   .2350   .1500   .1005   .0996   .1047   .0924   .1021        .1040
L. S. R VALUE     0.0000   .2903   .1916   .1345   .1445   .1549   .1348   .1470        .1409
R MODULUS         0.0000   .9843   .7051   .5286   .4928   .5070   .4792   .5867        .5393
R WEIGHTED        0.0000  1.4018   .6585   .4002   .4201   .4669   .4120   .5977        .4836
R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND        1
KRAUT R VALUE     0.0000   .2735   .2328   .1465   .1586   .1942   .1701   .1716        .1804
RATIO DELF/FPH      0.00     .46     .31     .19     .19     .21     .13     .21          .20
CENTRIC R VALUE   0.0000   .5970   .7572   .7902   .8880   .9183  1.2736   .8243        .8904
R MODULUS         0.0000  1.0714  1.3181  1.0594  1.0725  1.0993   .8148   .8734        .9873
 PT2 +HG EUREKA NO. 1 MAY 13 1975
COMPOUND 2     HG ANOM
MINIMUM ZONE SPACINGS FOR SHELLS
                    39.22   19.61   13.07    9.80    7.84    6.54    5.60    4.90
RMS CLOSURE         0.00  430.62  149.69  114.83   87.91   91.03   99.66  103.38
RMS EST. ERROR      0.00  176.09  232.87  290.79  319.23  322.96  356.19  419.05
RMS SMALLF          0.00  213.21  151.77  145.37  160.95  171.10  158.90  148.90
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NUM PER ZONE	0.	22.	72.	133.	210.	257.	266.	305.	
RMS DIFFERENCES	0.00	464.45	281.18	163.43	134.78	133.17	139.78	146.51	
A.D.RESIDUALS	0.00	3.93	4.72	6.34	6.58	6.56	7.28	8.71	
STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND					2				
NUM PER ZONE	0.0	22.0	72.0	133.0	210.0	257.0	266.0	305.0	1265.0
AVG LK OF CLOS	0.00	308.20	110.84	84.38	58.15	57.21	65.78	68.01	72.50
AVG DERIV FPH	0.00	853.57	816.59	882.34	862.11	770.19	740.15	826.34	808.55
AVG W*(E**2)	0.00	1.10	.60	.40	.33	.37	.41	.42	.42
AVG W*(FPH**2)	0.00	4.87	20.31	32.32	34.99	28.65	23.85	29.37	28.37
AVG SMALL F	0.00	196.48	135.66	130.33	144.38	152.02	137.73	132.28	140.63
AVG FP(NATIVE)	0.00	526.45	686.23	802.87	817.47	743.15	765.62	866.69	789.27
AVG W*(FH**2)	0.00	.27	.62	.77	1.09	1.31	1.04	.88	1.00
STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND					2				
NUM PER ZONE	0.0	11.0	23.0	39.0	39.0	47.0	44.0	44.0	247.0
AVG LK OF CLOS	0.00	401.87	133.74	122.42	120.61	128.58	111.07	150.70	139.82
AVG DERIV FPH	0.00	841.93	745.96	817.82	956.58	829.33	775.42	1001.98	861.56
AVG SMALL F	0.00	219.29	121.81	120.25	116.75	134.69	101.32	100.60	120.13
AVG FP(NATIVE)	0.00	500.98	694.72	731.97	937.76	820.44	788.84	1003.53	826.05
AVG DELF N.C.O.	0.00	402.75	119.58	145.93	133.10	126.04	125.98	150.64	146.39
AVG DELF C.O.	0.00	402.75	119.58	145.93	133.10	126.04	125.98	150.64	146.39
NUM CROSS OVERS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND					2				
KRAUT R VALUE	0.0000	.3612	.1455	.0956	.0675	.0743	.0889	.0823	.0897
L. S. R VALUE	0.0000	.4760	.1722	.1222	.0965	.1139	.1309	.1202	.1220
R MODULUS	0.0000	1.5691	.8760	.6474	.4014	.3763	.4776	.5142	.5156
R WEIGHTED	0.0000	4.0793	.9727	.6240	.2983	.2831	.3934	.4821	.4220
R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND					2				
KRAUT R VALUE	0.0000	.4773	.1793	.1497	.1261	.1550	.1432	.1504	.1623
RATIO DELF/FPH	0.00	.48	.16	.18	.14	.15	.16	.15	.17
CENTRIC R VALUE	0.0000	.9970	1.1185	.8389	.9062	1.0202	.8816	1.0004	.9551
R MODULUS	0.0000	1.8326	1.0979	1.0180	1.0331	.9547	1.0962	1.4980	1.1639

```
      PROGRAM LEASTSQ(DATA,FOUR,PUNCH,INPUT,OUTPUT,                     LEASTSQ01   1
     * TAPE1,TAPE2,TAPE3,TAPE4,                                         LEASTSQ01   2      MAIN PROGRAM
     * TAPE20=FOUR,TAPE14=DATA,TAPE5=INPUT,TAPE6=OUTPUT,TAPE7=PUNCH)    LEASTSQ01   3
C     MAIN PROGRAM FOR PHASE REFINEMENT                                 LEASTSQ     5
      DIMENSION RECIP(6),DDX(50,2),DDY(50,2),DDZ(50,2),DDR(50,6,2)      LEASTSQ     6
      DIMENSION DDANUM(50,6,2),DERIV(80),CORLAT(80),T(24,3,4)           LEASTSQ     7
      DIMENSION HDASH(24,4),TRIG(50,24,2),ST(2),OUT(9),ALPH(9)          LEASTSQ     8
      DIMENSION NPCYCL(16),TEPETI(18)                                   LEASTSQ     9
      COMMON/ATOMS/Q(8,10),Q1(8,10),BOVER(8,10),BOVR1(8,10),            LEASTSQ    10
     1 IFBOVR(8,10),ANUM(50,10),ANUM1(50,10),X(50),X1(50),Y(50),Y1(50),  LEASTSQ    11
     2 Z(50),Z1(50),R(50,6),R1(50,6),NTROP(50),LABEL(50,5),             LEASTSQ    12
     3 AMAGS,AMAGBO,AMAGX,AMAGY,AMAGZ,AMAGR,AMAGA,CPDTLE(8,2),          LEASTSQ    13
     4 CAY(8),NATOM(8),NCRYST(8),KK1(8),NZ(8,10)                        LEASTSQ    14
      COMMON/FINL/ TRIX(80,80),RHS(80),R(4,9),ECALC(8,9,9)              LEASTSQ    15
      COMMON/DATA/H(3),FNAT,F(8),ERR(8),AD(8),ERNAT,ADNAT,NNO,NNAT,     LEASTSQ    16
     1 NNHV(8),FAZRST,FAZMP,FIGMER,REAL(8),EMAG(8)                      LEASTSQ    17
      COMMON /DEVICE/ IIN, IOUT, INCARD, FMT(20),IOUT1,IOUT2,           LEASTSQ    18
     1 IOUT3,IOUT4,MMM,IM,IW,IP,ITT                                     LEASTSQ    19
      COMMON STAB(450),FTAB(450),NFS(8),RVAL(8,9,9),RCEN(8,9,9),        LEASTSQ    20
     1 TITLE(20),EIS(8,9),EAD(8,9),FSIZE(8,3),FIG(2,9),DSTRB(10),GAP    LEASTSQ    21
    2 FORMAT(2I5,F10.5,2A4)                                             LEASTSQ    22
 3    FORMAT(4I5,4F10.4,I5)                                             LEASTSQ    23
  4   FORMAT(3F10.4,I5,5X,5I1)                                          LEASTSQ    24
  5   FORMAT(12F3.0)                                                    LEASTSQ    25
  6   FORMAT(9F8.0)                                                     LEASTSQ    26
  7   FORMAT(6F10.6)                                                    LEASTSQ    27
 8    FORMAT(8F8.1)                                                     LEASTSQ    28
   60 FORMAT( 3I3, 1X, 7F9.3 )                                          LEASTSQ    29
 90   FORMAT(8I3)                                                       LEASTSQ    30
 94   FORMAT(1H 10F10.4)                                                LEASTSQ    31
 95   FORMAT(19H0CORRELATION MATRIX )                                   LEASTSQ    32
   97 FORMAT(1H1,20A4,///)                                              LEASTSQ    33
  98  FORMAT(20A4)                                                      LEASTSQ    34
 99   FORMAT(25H MORE THAM  80 VARIABLES )                              LEASTSQ    35
  103 FORMAT(/24H ERROR AFTER REFLECTION ,3F4.0/)                       LEASTSQ    36
  107 FORMAT(/42H END OF FILE ENCOUNTERED AFTER REFLECTION ,3F4.0/)     LEASTSQ    37
  109 FORMAT(16I5)                                                      LEASTSQ    38
  414 FORMAT(I5,F10.4,F10.4,I5)                                         LEASTSQ    39
  415 FORMAT(8F10.4)                                                    LEASTSQ    40
  516 FORMAT("0CRYSTAL NO.",I3,"  NZ(I,J)=",I3,/," SCALE =",F10.4,/,    LEASTSQ    41
     1" BOVER =",F10.4,"  IFBOVR =",I2)                                 LEASTSQ    42
  418 FORMAT("0ANUMS =",10F10.4)                                        LEASTSQ    43
  804 FORMAT(1H0," INPUT DATA FORMAT=", 20A4)                           LEASTSQ    44
  806 FORMAT(/," RECIP=", 6F10.5,/," DSTMAX=",F7.3, 5X," DSTMIN=",      LEASTSQ    45
     1 F7.3, 5X, " GAP=", F10.3,/)                                      LEASTSQ    46
  808 FORMAT(" NSYM=",I5,5X," NCPDS=",I5,5X," IANGLE=",I5,5X," NCYCLE=", LEASTSQ    47
     1  I5,/," SCALE=",F7.3,3X," FIGMIN=",F7.3,3X," FGAP=",F7.3,3X,     LEASTSQ    48
     2 " REJANO=",F7.3,3X," IFPRINT=",I5,/)                             LEASTSQ    49
  810 FORMAT( " NPCYCL=", 16I3)                                         LEASTSQ    50
  812 FORMAT( " SYMMETRY CARDS ",/, 3(4F6.2,3X) )                       LEASTSQ    51
  814 FORMAT( " FSIZF=",8F10.3,/)                                       LEASTSQ    52
  815 FORMAT("0COMPOUND ",I3,5X,2A4,/," NATOMS =",I5,/," NCRYST =",I5,/, LEASTSQ    53
     1" CAY =",F10.4,/)                                                 LEASTSQ    54
  816 FORMAT(" EIS=",8F10.3,/," EAD=", 8F10.3,/)                        LEASTSQ    55
  818 FORMAT(" COORDINATES =",3F7.4,/," NTROP=",I2,"   R =",6F10.3,/,   LEASTSQ    56
     1" LABEL =",5I3)                                                   LEASTSQ    57
  830 FORMAT(8F10.3)                                                    LEASTSQ    58
  835 FORMAT(1H ,"MAGNIFICATION FACTORS FOR SHIFTS ARE",/,1H ,          LEASTSQ    59
     1"FOR SCALE", F10.3,/,1H ,"FOR BOVER",F10.3,/,                     LEASTSQ    60
     2  1H ,"FOR ANUM ",F10.3,/," FOR X,Y,Z",3F10.3,/                   LEASTSQ    61
     3,1H ,"FOR B    ",F10.3)                                           LEASTSQ    62
C READ IN IIN,IOUT,INCARD DATA FORMAT DATA CARDS IF APPROPRIATE         LEASTSQ    63
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      CALL IOSET                                                        LEASTSQ    64
      UNIT=1.0                                                          LEASTSQ    67
C  MAKE SINE TABLE                                                      LEASTSQ    68
      DO 53 I=1,450                                                     LEASTSQ    69
 53   STAB(I)=SIN(FLOAT(I)*0.017453)                                    LEASTSQ    70
C MAKE EXPONENTIAL TABLE                                                LEASTSQ    71
      DO 54 I=1,450                                                     LEASTSQ    72
      X(1)=FLOAT(I-1)/150.0                                             LEASTSQ    73
   54 ETAB(I)=EXP(-0.5*X(1)*X(1))                                       LEASTSQ    74
      DO 74 I=1,8                                                       LEASTSQ    75
      DO 74 J=1,10                                                      LEASTSQ    76
   74 Q(I,J)=0.0                                                        LEASTSQ    77
C                                                                       LEASTSQ    78
C A  READ IN CONTROL CARDS                                              LEASTSQ    79
C                                                                       LEASTSQ    80
      READ(IM,98)  ( TITLE(I),I=1,20)                                   LEASTSQ    81
      WRITE(IW,97)  ( TITLE(I),I=1,20)                                  LEASTSQ    82
      READ(IM,6)  ( RECIP(I),I=1,6),DSTMAX,DSTMIN,GAP                   LEASTSQ    83
C                                                                       LEASTSQ02   1
C     IF REAL CELL GIVEN, CONVERT TO RECIP                              LEASTSQ02   2
C                                                                       LEASTSQ02   3
      IF(RECIP(1).GT.1.)CALL CONRCP(RECIP,RECIP)                        LEASTSQ02   4
      IF(GAP.EQ.0.0) GAP=0.1/1.542                                      LEASTSQ    84
      READ(IM,3)NSYM,NCPDS,IANGLE,NCYCLE,SCALE,FIGMIN,FGAP,REJANO,IFPRNT LEASTSQ    85
      READ(IM,830)AMAGS,AMAGRO,AMAGA,AMAGX,AMAGY,AMAGZ,AMAGB            LEASTSQ    86
      WRITE(IW,835)  AMAGS,AMAGRO,AMAGA,AMAGX,AMAGY,AMAGZ,AMAGB         LEASTSQ    87
      READ(IM,90)(NFS(I),I=1,8)                                         LEASTSQ    88
      READ 109, NPCYCL                                                  LEASTSQ    89
      DO 110 IJKL=1,16                                                  LEASTSQ    90
      IF(NPCYCL(IJKL).LE.0.OR.NPCYCL(IJKL).GE.10)NPCYCL(IJKL)=1         LEASTSQ    91
  110 CONTINUE                                                          LEASTSQ    92
      DO 14 N=1,NSYM                                                    LEASTSQ    93
 14   READ(IM,5)((T(N,I,J),J=1,4),I=1,3)                                LEASTSQ    94
      READ   8,(FSIZE(J,2),J=1,8)                                       LEASTSQ    95
      WRITE(IW,806)(RECIP(I),I=1,6), DSTMAX,DSTMIN, GAP                 LEASTSQ    96
      WRITE(IW,808)NSYM, NCPDS, IANGLE, NCYCLE, SCALE, FIGMIN, FGAP,    LEASTSQ    97
     1   REJANO, IFPRNT                                                 LEASTSQ    98
      WRITE(IW,810)( NPCYCL(JJ),JJ=1,16)                                LEASTSQ    99
      PRINT 812,  ((( T(N,I,J),J=1,4),I=1,3),N=1,NSYM)                  LEASTSQ   100
      WRITE(IW,814)(FSIZE(J,2),J=1,8)                                   LEASTSQ   101
      NVAR=0                                                            LEASTSQ   102
      LIST=0                                                            LEASTSQ   103
      DO 10 I=1,NCPDS                                                   LEASTSQ   104
      WRITE(IW,97)TITLE                                                 LEASTSQ   105
      READ(IM,2)NATOM(I),NCRYST(I),CAY(I),CPDTLE(I,1),CPDTLE(I,2)       LEASTSQ   106
      READ(IM,8)(EIS(I,J),J=1,8)                                        LEASTSQ   107
      READ(IM,8)(EAD(I,J),J=1,8)                                        LEASTSQ   108
      N=NATOM(I)                                                        LEASTSQ   109
      WRITE(IW,815)I,CPDTLE(I,1),CPDTLE(I,2),NATOM(I),NCRYST(I),CAY(I)  LEASTSQ   110
      WRITE(IW,816)( EIS(I,J),J=1,8), ( EAD(I,J),J=1,8)                 LEASTSQ   111
      M=NCRYST(I)                                                       LEASTSQ   112
      DO 413 J=1,M                                                      LEASTSQ   113
      READ(IM,414)NZ(I,J),SCL,BOVER(I,J),IFBOVR(I,J)                    LEASTSQ   114
      WRITE(IW,516)J,NZ(I,J),SCL,BOVER(I,J),IFBOVR(I,J)                 LEASTSQ   115
      Q(I,J) = 1.0/SCL                                                  LEASTSQ   116
  413 NVAR = NVAR+1+IFBOVR(I,J)                                         LEASTSQ   117
      DO 13 J=1,N                                                       LEASTSQ   118
      LIST=LIST+1                                                       LEASTSQ   119
      READ(IM,415)(ANUM(LIST,K),K=1,M)                                  LEASTSQ   120
      READ(IM,4)            X(LIST),Y(LIST),Z(LIST),NTROP(LIST),        LEASTSQ   121
     1(LABEL(LIST,K),K=1,5)                                             LEASTSQ   122
      READ(IM,7)(B(LIST,K),K=1,6)                                       LEASTSQ   123
```

Title

a^{*2} b^{*2} c^{*2} $2a^*b^*\cos\gamma^*$

$2b^*c^*\cos\alpha^*$ $2c^*a^*\cos\beta^*$

= RECIP(1) − RECIP(6)

d^*_{max} d^*_{min} gap

n_{sym} n_{cpd} $\Delta\alpha_i$ n_{cycl} SCALE

$\bar{m}_{min}$ F_{gap} REJANO IFPRNT

Magnification factors

NFS

NPCYCL if NPCYC ≤ 0 or ≥ 10 put equal to 1

(t(n,i,j),j=1,4)i=1,3)n=1,n_{sym}

FSIZE

#HA1,#CRYST,CAY,TITLE

E_{IS}

E_{AD}

NZ SCL BOVER BOVR

Q_{ij} = 1/SCL

Z x y z B or β

NVAR = # variables

= 1 + 1 (if BOVER refined)

+ # xyz refined + # TF refined

+ # atoms with scale refined

```
      WRITE(IW,418)(ANUM(LIST,K),K=1,M)
      WRITE(IW,818)            X(LIST),Y(LIST),Z(LIST),NTROP(LIST),
     1 (B(LIST,K),K=1,6),(LABEL(LIST,K),K=1,5)
      DO 62 K=2,4
 62   NVAR=NVAR+LABEL(LIST,K)
      NVAR=NVAR+LABEL(LIST,5)*NTROP(LIST)
      NVAR = NVAR + LABEL(LIST,1)*M
 13   CONTINUE
 10   CONTINUE
C
C A END
C
      IF(NVAR.LE. 80) GO TO 11
      WRITE(IW,99)
      STOP
 11   CONTINUE
      DO 822 J=1,NCPDS
      M=NCRYST(J)
      DO 822 I=1,M
      Q1(J,I) = 1.0/Q(J,I)
      BOVR1(J,I) = BOVER(J,I)
 822  CONTINUE
      DO 820 J=1,LIST
      X1(J) = X(J)
      Y1(J) = Y(J)
      Z1(J) = Z(J)
      DO 820 K=1,6
      B1(J,K) = B(J,K)
      ANUM1(J,K) = ANUM(J,K)
 820  CONTINUE
      IF(IOUT.NE.IP.AND.IOUT.NE.0)REWIND IOUT
      DO 18 J=1,8
 18   FSIZE(J,3)=FSIZE(J,2)*FSIZE(J,2)
C
C B EACH NEW CYCLE STARTS HERE
C
      DO 50 ICYCLE=1,NCYCLE
      MARK=NCYCLE-ICYCLE
      NTHCYC=NPCYCL(ICYCLE)
C
C C CONTROL ON INDIVIDUAL CYCLE
C
      DO 50 NUMCYC=1,NTHCYC
      REWIND IIN
      DO 41 M=1,NVAR
      DO 42 N=1,NVAR
 42   TRIX(M,N)=0.0
 41   RHS(M)=0.0
      DO 12 I=1,4
      DO 12 J=1,9
 12   R(I,J)=0.0
      DO 17 I=1,8
      DO 17 J=1,9
      DO 17 K=1,9
      RVAL(I,J,K)=0.0
      RCEN(I,J,K)=0.0
 17   ECALC(I,J,K)=0.0
      DO 22 J=1,2
      DO 22 K=1,9
 22   FIG(J,K)=0.0
      DO 23 I=1,10
 23   DSTRB(I)=0.0
```

E_{is} = rms lack of closure in shells of GAP, i.e. as a function of 1/d for each isomorphous compound

FSIZE = rms lack of closure in shells of FGAP, i.e. as a function of F_{native}

FSIZE(j,3) = $\{\text{FSIZE}(j,2)\}^2$ input

Cycle the program for the required # of cycles

MARK = # cycles left to do

NTHCYC = 1 '.' NPCYCL = 1

Clear areas

```
      DO 19 J=1,8                                                       LEASTSQ   186
      DO 19 K=1,2                                                       LEASTSQ   187
 19   FSIZE(J,K)=0.0                                                    LEASTSQ   188
C                                                                       LEASTSQ   189
C D EACH NEW BLOCK OF DATA STARTS HERE                                  LEASTSQ   190
C                                                                       LEASTSQ   191
   15 CONTINUE                                                          LEASTSQ   192
      CALL TAPEIN(IIN,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP,  LEASTSQ05    1
     * FIGMER,NNHV,F,ERR,AD)                                            LEASTSQ05    2
      IF(IFPRNT.GT.1)                                                   LEASTSQ01    4
     *WRITE(IW,8835)NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,                 LEASTSQ01    5
     *FAZBST,FAZMP,FIGMER,((NNHV(II3),F(II3),ERR(II3),AD(II3)),II3=1,8) LEASTSQ01    6
 8835 FORMAT(1X,4I4,I5,6E15.8/,8(1X,I10,3E15.8/))                       LEASTSQ01    7
      IF(NNO.EQ.0) GO TO 105                                            LEASTSQ   197
      H(1)=IH                                                           LEASTSQ   198
      H(2)=IK                                                           LEASTSQ   199
      H(3)=IL                                                           LEASTSQ   200
      DO 999 II10=1,8                                                   LEASTSQ   201
       IF(ABS(AD(II10)).GE.REJANO) AD(II10)=0.0                         LEASTSQ   202
  999 CONTINUE                                                          LEASTSQ   203
      GO TO 106                                                         LEASTSQ   204
  102 DO 104 II7=1,3                                                    LEASTSQ   205
  104 H(II7)= 999.                                                      LEASTSQ   206
      NNAT=0                                                            LEASTSQ   207
      FNAT=-1.0                                                         LEASTSQ   208
      PRINT 103,(H(II2),II2=1,3)                                        LEASTSQ   209
      GO TO 15                                                          LEASTSQ   210
  105 PRINT 107,(H(II2),II2=1,3)                                        LEASTSQ   211
      DO 108 II7=1,3                                                    LEASTSQ   212
  108 H(II7)=999.                                                       LEASTSQ   213
      NNO=0                                                             LEASTSQ   214
      FNAT=-2.0                                                         LEASTSQ   215
      IH=999                                                            LEASTSQ   216
      IK=999                                                            LEASTSQ   217
      IL=999                                                            LEASTSQ   218
      ZRO=0.                                                            LEASTSQ   219
      IF(MARK.NE.0) GO TO 489                                           LEASTSQ   220
      IF(IOUT3.NE.0) WRITE(IOUT3) IH,IK,IL,ZRO,ZRO,ZRO,ZRO,ZRO          LEASTSQ   221
      IF(IOUT3.NE.0) END FILE IOUT3                                     LEASTSQ   222
      IF(IOUT4.NE.0) WRITE(IOUT4) IH,IK,IL,ZRO,ZRO,ZRO,ZRO,ZRO          LEASTSQ   223
      IF(IOUT4.NE.0) END FILE IOUT4                                     LEASTSQ   224
  489 CONTINUE                                                          LEASTSQ   225
      IF(NUMCYC.NE.1) GO TO 89                                          LEASTSQ   226
      IF(IOUT1.EQ.0) GO TO 89                                           LEASTSQ   227
      CALL TAPOUT(IOUT1,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP, LEASTSQ05    3
     * FIGMER,NNHV,F,ERR,AD)                                            LEASTSQ05    4
      END FILE IOUT1                                                    LEASTSQ   230
      IIN=IOUT1                                                         LEASTSQ   231
      IOUT1=IOUT2                                                       LEASTSQ   232
      IOUT2=IIN                                                         LEASTSQ   233
      REWIND IOUT1                                                      LEASTSQ   234
      GO TO 89                                                          LEASTSQ   235
  106 CONTINUE                                                          LEASTSQ   236
      IF(NNAT.NE.0) GO TO 416                                           LEASTSQ   237
 417  IF(IOUT1.NE.0)CALL TAPOUT(IOUT1,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT LEASTSQ05    5
     * ,FAZBST,FAZMP,FIGMER,NNHV,F,ERR,AD)                              LEASTSQ05    6
      GO TO 15                                                          LEASTSQ   240
  416 CONTINUE                                                          LEASTSQ   241
      ALPHA=FAZMP                                                       LEASTSQ   242
      DSTSQ=H(1)*H(1)*RECIP(1)+H(2)*H(2)*RECIP(2)+H(3)*H(3)*RECIP(3)+   LEASTSQ   243
     1  H(1)*H(2)*RECIP(4)+H(2)*H(3)*RECIP(5)+H(1)*H(3)*RECIP(6)        LEASTSQ   244
      DST=SQRT(DSTSQ)                                                   LEASTSQ   245
```

Call data on tape

If AD > REJANO, AD = 0

End of file

Which files to be written on when data all read

Output

α = FAZMP

d^* computed from RECIP(1)-RECIP(6) (r_1-r_6) and hkl.

$$d^* = \sqrt{h^2 r_1 + k^2 r_2 + \ell^2 r_3 + hk r_4 + k\ell r_5 + \ell h r_6}$$

Check that this lies between d^*_{max} and d^*_{min}

NORDER defines the shell specified by GAP

d^* in units of $\mathring{A}^{-1}$ $\left(\frac{d^*}{gap} + 1\right)$ defines the shell.

```
      IF((DST.GT.DSTMAX).OR.(DST.LT.DSTMIN)) GO TO 417                  LEASTSQ   246
      NORDER=1+IFIX(DST/GAP)                                            LEASTSQ   247
      IF(NORDER.GT.8) NORDER=8                                          LEASTSQ   248
      DO 25 J=1,NSYM                                                    LEASTSQ   249
      DO 25 K=1,4                                                       LEASTSQ   250
 25   HDASH(J,K)=T(J,1,K)*H(  1)+T(J,2,K)*H(  2)+T(J,3,K)*H(  3)        LEASTSQ   251
      DO 26 L=1,LIST                                                    LEASTSQ   252
      DO 26 J=1,NSYM                                                    LEASTSQ   253
      ANGLE=HDASH(J,1)*X(L)+HDASH(J,2)*Y(L)+HDASH(J,3)*Z(L)+HDASH(J,4)  LEASTSQ   254
      KUT=IFIX(ABS(ANGLE))                                              LEASTSQ   255
      JA=IFIX((ABS(ANGLE)-FLOAT(KUT))*360.0)                            LEASTSQ   256
      IF(JA.LE.0) JA=JA+360                                             LEASTSQ   257
      IF(JA.GT.360) JA=JA-360                                           LEASTSQ   258
      TRIG(L,J,1)=STAR(JA+90)                                           LEASTSQ   259
      IF(ANGLE.LT.0.0) GO TO 21                                         LEASTSQ   260
      TRIG(L,J,2)=STAR(JA)                                              LEASTSQ   261
      GO TO 26                                                          LEASTSQ   262
 21   TRIG(L,J,2)=-STAR(JA)                                             LEASTSQ   263
 26   CONTINUE                                                          LEASTSQ   264
      DO 32 L=1,LIST                                                    LEASTSQ   265
      DO 32 IS=1,2                                                      LEASTSQ   266
      DDX(L,IS)=0.0                                                     LEASTSQ   267
      DDY(L,IS)=0.0                                                     LEASTSQ   268
      DDZ(L,IS)=0.0                                                     LEASTSQ   269
      DO 32 IC=1,6                                                      LEASTSQ   270
      DDANUM(L,IC,IS) = 0.0                                             LEASTSQ   271
 32   DDB(L,IC,IS)=0.0                                                  LEASTSQ   272
      L=1                                                               LEASTSQ   273
C                                                                       LEASTSQ   274
C E CALCULATES TRIGONOMETRIC TERMS OF DERIVATIVES ON TEMPERATURE FACTOR, LEASTSQ   275
C     X, Y, Z AND ATOMIC NUMBER                                         LEASTSQ   276
C                                                                       LEASTSQ   277
      DO 24 M=1,NCPDS                                                   LEASTSQ   278
      MCPD=NFS(M)                                                       LEASTSQ   279
      REAL(M)=0.0                                                       LEASTSQ   280
      EMAG(M)=0.0                                                       LEASTSQ   281
      N=NATOM(M)                                                        LEASTSQ   282
      NN1 = NCRYST(M)                                                   LEASTSQ   283
      DO 27 K=1,N                                                       LEASTSQ   284
      KK1(M)=0                                                          LEASTSQ   285
      IF(NNHV(MCPD).EQ.0) GO TO 79                                      LEASTSQ   286
      DO 420 K1 =1,NN1                                                  LEASTSQ   287
      IF(NNHV(MCPD).EQ.NZ(M,K1)) GO TO 422                              LEASTSQ   288
  420 CONTINUE                                                          LEASTSQ   289
      KK1(M)=0                                                          LEASTSQ   290
      WRITE(IW,510) M,K1,MCPD                                           LEASTSQ01   8
510   FORMAT(" REJECTION ",3I5)                                         LEASTSQ   292
      GO TO 79                                                          LEASTSQ   293
  422 KK1(M)=K1                                                         LEASTSQ   294
      RQUIV=0.0                                                         LEASTSQ   295
      EQUIV=0.0                                                         LEASTSQ   296
      DO 28 J=1,NSYM                                                    LEASTSQ   297
      IF(NTROP(L).EQ.6) GO TO 29                                        LEASTSQ   298
      SCAT=ANUM(L,K1)*EXP(-B(L,1)*0.25*DSTSQ)                           LEASTSQ   299
      ST(1)=SCAT*TRIG(L,J,1)                                            LEASTSQ   300
      ST(2)=SCAT*TRIG(L,J,2)                                            LEASTSQ   301
      IF(LABEL(L,5).EQ.0) GO TO 30                                      LEASTSQ   302
      DDB(L,1,1)=DDB(L,1,1)-(0.25*DSTSQ*ST(1))                          LEASTSQ   303
      DDB(L,1,2)=DDB(L,1,2)-(0.25*DSTSQ*ST(2))                          LEASTSQ   304
      GO TO 30                                                          LEASTSQ   305
 29   SCAT=ANUM(L,K1)*EXP(-B(L,1)*HDASH(J,1)*HDASH(J,1)                 LEASTSQ   306
     1-B(L,2)*HDASH(J,2)*HDASH(J,2)-B(L,3)*HDASH(J,3)*HDASH(J,3)        LEASTSQ   307
```

For symmetry of space group $j=1\cdots n_{sym}$ and $k=1,4$

$h'_{jk} = t_{j1k}h + t_{j2k}k + t_{j3k}\ell$

angle $= h'_{j1}x + h'_{j2}y + h'_{j3}z + h'_{j4}$

This is set to be between 0 and 1 cycles

TRIG(L,J,1) = cos(2π(hx+ky+ℓz))
TRIG(L,J,2) = sin(2π(hx+ky+ℓz))
J = which asymmetric unit
L = which atom in the list

If NNHV(MCPD) ≠ any NZ(M,K1) then reject the reflection

CALCULATE "DERIVATIVES" FOR HEAVY ATOM REFINEMENT

$SCAT = Z_n \exp(-Bd^{*2}/4) = Z_n \exp(-B\sin^{2\theta}/\lambda^2)$
ST(1) = SCAT(cos 2π(hx+ky+ℓz))
ST(2) = SCAT(sin 2π(hx+ky+ℓz))

If isotopic, derivatives are:

$$DDB(L,1,1) = \Sigma-\left(\frac{\sin^2\theta}{\lambda^2}\right)ST(1)$$

$$DDB(L,1,2) = \Sigma-\left(\frac{\sin^2\theta}{\lambda^2}\right)ST(2)$$

If anisotropic

$$SCAT = Z_n(\exp(-\beta_{11}(h')^2 - \beta_{22}(k')^2 -\beta_{33}(\ell')^2 - \beta_{12}(h'k') - \beta_{23}(k'\ell') -\beta_{31}(\ell'h')))$$

```
     2-B(L,4)*HDASH(J,1)*HDASH(J,2)-B(L,5)*HDASH(J,2)*HDASH(J,3)          LEASTSQ   308
     3-B(L,6)*HDASH(J,3)*HDASH(J,1))                                      LEASTSQ   309
      ST(1)=SCAT*TRIG(L,J,1)                                              LEASTSQ   310
      ST(2)=SCAT*TRIG(L,J,2)                                              LEASTSQ   311
      IF(LABEL(L,5).EQ.0) GO TO 30                                        LEASTSQ   312
      DO 31 IS=1,2                                                        LEASTSQ   313
      DDB(L,1,IS)=DDB(L,1,IS)-HDASH(J,1)*HDASH(J,1)*ST(IS)                LEASTSQ   314
      DDB(L,2,IS)=DDB(L,2,IS)-HDASH(J,2)*HDASH(J,2)*ST(IS)                LEASTSQ   315
      DDB(L,3,IS)=DDB(L,3,IS)-HDASH(J,3)*HDASH(J,3)*ST(IS)                LEASTSQ   316
      DDB(L,4,IS)=DDB(L,4,IS)-HDASH(J,1)*HDASH(J,2)*ST(IS)                LEASTSQ   317
      DDB(L,5,IS)=DDB(L,5,IS)-HDASH(J,2)*HDASH(J,3)*ST(IS)                LEASTSQ   318
 31   DDB(L,6,IS)=DDB(L,6,IS)-HDASH(J,3)*HDASH(J,1)*ST(IS)                LEASTSQ   319
 30   RQUIV=RQUIV+ST(1)                                                   LEASTSQ   320
      EQUIV=EQUIV+ST(2)                                                   LEASTSQ   321
      ST(1)=6.2832*ST(1)                                                  LEASTSQ   322
      ST(2)=6.2832*ST(2)                                                  LEASTSQ   323
      IF(LABEL(L,2).EQ.0) GO TO 63                                        LEASTSQ   324
      DDX(L,1)=DDX(L,1)-HDASH(J,1)*ST(2)                                  LEASTSQ   325
      DDX(L,2)=DDX(L,2)+HDASH(J,1)*ST(1)                                  LEASTSQ   326
 63   IF(LABEL(L,3).EQ.0) GO TO 64                                        LEASTSQ   327
      DDY(L,1)=DDY(L,1)-HDASH(J,2)*ST(2)                                  LEASTSQ   328
      DDY(L,2)=DDY(L,2)+HDASH(J,2)*ST(1)                                  LEASTSQ   329
 64   IF(LABEL(L,4).EQ.0) GO TO 28                                        LEASTSQ   330
      DDZ(L,1)=DDZ(L,1)-HDASH(J,3)*ST(2)                                  LEASTSQ   331
      DDZ(L,2)=DDZ(L,2)+HDASH(J,3)*ST(1)                                  LEASTSQ   332
 28   CONTINUE                                                            LEASTSQ   333
      IF(LABEL(L,1).EQ.0) GO TO 65                                        LEASTSQ   334
      DDANUM(L,K1,1)=RQUIV/ ANUM(L,K1)                                    LEASTSQ   335
      DDANUM(L,K1,2)=EQUIV/ ANUM(L,K1)                                    LEASTSQ   336
 65   REAL(M)=REAL(M)+RQUIV                                               LEASTSQ   337
      EMAG(M)=EMAG(M)+EQUIV                                               LEASTSQ   338
 79   L=L+1                                                               LEASTSQ   339
 27   CONTINUE                                                            LEASTSQ   340
 24   CONTINUE                                                            LEASTSQ   341
C                                                                         LEASTSQ   342
 D END                                                                    LEASTSQ   343
C                                                                         LEASTSQ   344
      II=I                                                                LEASTSQ   345
      IF(NUMCYC.EQ.1)  CALL PHASE(I,ALPHA,SCALE,NCPDS,IANGLE,CAY,FIGMIN,  LEASTSQ   346
     1 UNIT,IFPRNT,NORDER,MARK,Q,DSTSQ,BOVER,KK1)                         LEASTSQ   347
      I=II                                                                LEASTSQ   348
      FP=FNAT   *SCALE                                                    LEASTSQ   349
      IF(ALPHA.EQ.-10.0) GO TO 16                                         LEASTSQ   350
      FPSQ=FP*FP                                                          LEASTSQ   351
      FPA=FP*COS(ALPHA)                                                   LEASTSQ   352
      FPB=FP*SIN(ALPHA)                                                   LEASTSQ   353
      NV=1                                                                LEASTSQ   354
      L=1                                                                 LEASTSQ   355
C                                                                         LEASTSQ   356
C F ACCUMULATE VARIOUS VALUES FOR VARIOUS R FACTORS                       LEASTSQ   357
C                                                                         LEASTSQ   358
      DO 34 M=1,NCPDS                                                     LEASTSQ   359
      MCPD=NFS(M)                                                         LEASTSQ   360
      DO 33 MM=1,NVAR                                                     LEASTSQ   361
 33   DERIV(MM)=0.0                                                       LEASTSQ   362
      K1=KK1(M)                                                           LEASTSQ   363
      IF(KK1(M).EQ.0) GO TO 459                                           LEASTSQ   364
      QT=Q(M,K1)*EXP(BOVER(M,K1)*DSTSQ*0.25)                              LEASTSQ   365
      AX=REAL(M)+FPA                                                      LEASTSQ   366
      BY=EMAG(M)+FPB                                                      LEASTSQ   367
      DE=QT   *SQRT(AX*AX+BY*BY)                                          LEASTSQ   368
      EPSILN=F(   MCPD)-DE                                                LEASTSQ   369
```

ST(1) and ST(2) defined above

$DDX(L,1) = -\Sigma(h'_{J1})ST(2)$

$DDX(L,2) = +\Sigma(h'_{J1})ST(1)$

$DDY(L,1) = -\Sigma(h'_{J2})ST(2)$

$DDY(L,2) = +\Sigma(h'_{J2})ST(1)$

$DDZ(L,1) = -\Sigma(h'_{J3})ST(2)$

$DDZ(L,2) = +\Sigma(h'_{J3})ST(1)$

$DDANUM(L,K1,1) = (1/Z_n)(\Sigma ST(1))$

$DDANUM(L,K1,2) = (1/Z_n)(\Sigma ST(2))$

$REAL(M) = \Sigma RQUIV = \Sigma\Sigma ST(1) = A_{HA}$

$EMAG(M) = \Sigma EQUIV = \Sigma\Sigma ST(2) = B_{HA}$

These calculations are made for all derivatives

Call the PHASE subroutine

$FP = SCALE * FNAT$

$FPA = FP * \cos(\phi_{max}) = A_P$

$FPB = FP * \sin(\phi_{max}) = B_P$

$QT = Q_{m,K1} \exp(BOVER * \sin^2\theta/\lambda^2)$

$= (SHAPE/SCL)$

$AX = A_{HA} + A_P = A_{PHcalc}$

$BX = B_{HA} + B_P = B_{PHcalc}$

$DE = (SHAPE/SCL) * F_{PHcalc}$

$EPSILN = F_{PHobs} - (SHAPE/SCL) * F_{PHcalc}$

$EPNSQ = (EPSILN)^2$

$EPS = (SCL/SHAPE) * F_{PHobs} - F_{PHcalc}$

$EPSQ = (EPS)^2$

```
      EPNSQ=EPSILN*FPSILN                                               LEASTSQ   370
      EPS=EPSILN/QT                                                     LEASTSQ   371
      EPSQ=EPS*EPS                                                      LEASTSQ   372
      NS=1+IFIX(FP/FGAP)                                                LEASTSQ   373
      IF(NS.GT.8) NS=8                                                  LEASTSQ   374
      W=1.0/(QT  *QT  *(EIS(M,NORDER)*EIS(M,NORDER)+FSIZE(NS,3))*1.0E6) LEASTSQ   375
      CONST=(QT  *QT  )/DE                                              LEASTSQ   376
      AXCON=CONST*AX                                                    LEASTSQ   377
      BYCON=CONST*BY                                                    LEASTSQ   378
      FFSQ=REAL(M)*REAL(M)+EMAG(M)*EMAG(M)                              LEASTSQ   379
      FF=SQRT(FFSQ)                                                     LEASTSQ   380
      R(1,NORDER)=R(1,NORDER)+ABS(EPS)                                  LEASTSQ   381
      R(2,NORDER)=R(2,NORDER)+FF                                        LEASTSQ   382
      R(3,NORDER)=R(3,NORDER)+W*EPNSQ                                   LEASTSQ   383
      R(4,NORDER)=R(4,NORDER)+W*(FFSQ*(QT  **2))                        LEASTSQ   384
      R(1,9)=R(1,9)+ABS(EPS)                                            LEASTSQ   385
      R(2,9)=R(2,9)+FF                                                  LEASTSQ   386
      R(3,9)=R(3,9)+W*EPNSQ                                             LEASTSQ   387
      R(4,9)=R(4,9)+W*(FFSQ*(QT  **2))                                  LEASTSQ   388
      RVAL(M,1,NORDER)=RVAL(M,1,NORDER)+1.0                             LEASTSQ   389
      RVAL(M,2,NORDER)=RVAL(M,2,NORDER)+ABS(EPS)                        LEASTSQ   390
      RVAL(M,3,NORDER)=RVAL(M,3,NORDER)+ABS(F(  MCPD)/QT  )             LEASTSQ   391
      RVAL(M,4,NORDER)=RVAL(M,4,NORDER)+W*EPNSQ*1.0E6                   LEASTSQ   392
      RVAL(M,5,NORDER)=RVAL(M,5,NORDER)+W*(F(  MCPD)**2)*1.0E6          LEASTSQ   393
      RVAL(M,6,NORDER)=RVAL(M,6,NORDER)+ABS(FF)                         LEASTSQ   394
      RVAL(M,7,NORDER)=RVAL(M,7,NORDER)+ABS(FP)                         LEASTSQ   395
      RVAL(M,8,NORDER)=RVAL(M,8,NORDER)+W*(FFSQ*(QT  **2))*1.0E6        LEASTSQ   396
      RVAL(M,1,9)=RVAL(M,1,9)+1.0                                       LEASTSQ   397
      RVAL(M,2,9)=RVAL(M,2,9)+ABS(EPS)                                  LEASTSQ   398
      RVAL(M,3,9)=RVAL(M,3,9)+ABS(F(  MCPD)/QT  )                       LEASTSQ   399
      RVAL(M,4,9)=RVAL(M,4,9)+W*EPNSQ*1.0E6                             LEASTSQ   400
      RVAL(M,5,9)=RVAL(M,5,9)+W*(F(  MCPD)**2)*1.0E6                    LEASTSQ   401
      RVAL(M,6,9)=RVAL(M,6,9)+ABS(FF)                                   LEASTSQ   402
      RVAL(M,7,9)=RVAL(M,7,9)+ABS(FP)                                   LEASTSQ   403
      RVAL(M,8,9)=RVAL(M,8,9)+W*(FFSQ*(QT  **2))*1.0E6                  LEASTSQ   404
C                                                                       LEASTSQ   405
C     CHECK TO SEE IF CENTRIC ZONE OF SPACE GROUP                       LEASTSQ   406
      IF(CENZON(H).NE.0.)GO TO 111                                      LEASTSQ01   9
      RCEN(M,1,NORDER)=RCEN(M,1,NORDER)+1.0                             LEASTSQ   409
      RCEN(M,2,NORDER)=RCEN(M,2,NORDER)+ABS(EPS)                        LEASTSQ   410
      RCEN(M,3,NORDER)=RCEN(M,3,NORDER)+ABS(F(  MCPD)/QT  )             LEASTSQ   411
      RCEN(M,4,NORDER)=RCEN(M,4,NORDER)+ABS(ABS(FP)-ABS(F(  MCPD)/QT  )) LEASTSQ   412
      RCEN(M,6,NORDER)=RCEN(M,6,NORDER)+ABS(FF)                         LEASTSQ   413
      RCEN(M,7,NORDER)=RCEN(M,7,NORDER)+ABS(FP)                         LEASTSQ   414
      RCEN(M,1,9)=RCEN(M,1,9)+1.0                                       LEASTSQ   415
      RCEN(M,2,9)=RCEN(M,2,9)+ABS(EPS)                                  LEASTSQ   416
      RCEN(M,3,9)=RCEN(M,3,9)+ABS(F(  MCPD)/QT  )                       LEASTSQ   417
      RCEN(M,4,9)=RCEN(M,4,9)+ABS(ABS(FP)-ABS(F(  MCPD)/QT  ))          LEASTSQ   418
      RCEN(M,6,9)=RCEN(M,6,9)+ABS(FF)                                   LEASTSQ   419
      RCEN(M,7,9)=RCEN(M,7,9)+ABS(FP)                                   LEASTSQ   420
      IF(FP.EQ.0.0) GO TO 112                                           LEASTSQ   421
      IF((AX/FPA).LT.0.0) GO TO 113                                     LEASTSQ   422
  112 RCEN(M,5,NORDER)=RCEN(M,5,NORDER)+ABS(ABS(FP)-ABS(F(  MCPD)/QT  )) LEASTSQ   423
      RCEN(M,5,9)=RCEN(M,5,9)+ABS(ABS(FP)-ABS(F(  MCPD)/QT  ))          LEASTSQ   424
      GO TO 111                                                         LEASTSQ   425
  113 RCEN(M,5,NORDER)=RCEN(M,5,NORDER)+ABS(ABS(FP)+ABS(F(  MCPD)/QT  )) LEASTSQ   426
      RCEN(M,8,NORDER)=RCEN(M,8,NORDER)+1.0                             LEASTSQ   427
      RCEN(M,5,9)=RCEN(M,5,9)+ABS(ABS(FP)+ABS(F(  MCPD)/QT  ))          LEASTSQ   428
      RCEN(M,8,9)=RCEN(M,8,9)+1.0                                       LEASTSQ   429
  111 CONTINUE                                                          LEASTSQ   430
      ECALC(M,1,NORDER)=ECALC(M,1,NORDER)+EPSQ                          LEASTSQ   431
      ECALC(M,2,NORDER)=ECALC(M,2,NORDER)+FFSQ                          LEASTSQ   432
```

$$NS = \text{shell by } F_{gap} = 1 + \frac{F_P}{F_{gap}}$$

$$\text{Weight} = W = 1.0/\{(SHAPE/SCL)^2\ \{(E_{1S})^2 + (FSIZE)^2\}\}$$

$$CONST = \left(\frac{SHAPE}{SCL}\right) * \frac{1}{F_{PHcalc}}$$

$$AXCON = \left(\frac{SHAPE}{SCL}\right) * \left(\frac{A_{PHcalc}}{F_{PHcalc}}\right) = \cos\alpha_{PHcalc}$$

$$BYCON = \left(\frac{SHAPE}{SCL}\right) * \left(\frac{B_{PHcalc}}{F_{PHcalc}}\right) = \sin\alpha_{PHcalc}$$

$$FFSQ = f_j^2 = (FSMALL)^2 = (FF)^2$$

Get ready for R values

```
      ECALC(M,3,NORDER)=ECALC(M,3,NORDER)+1.0                           LEASTSQ   433
      ECALC(M,4,NORDER)=ECALC(M,4,NORDER)+(((F(   MCPD)/QT   )-FP)**2)  LEASTSQ   434
      ECALC(M,9,NORDER)=ECALC(M,9,NORDER)+((ERNAT    *SCALF)**2+       LEASTSQ   435
     1 (ERR(   MCPD)/QT   )**2)                                         LEASTSQ   436
      IF(CAY(M).EQ.0) GO TO 20                                          LEASTSQ   437
C                                                                       LEASTSQ   438
C     CHECK FOR CENTRIC ZONE OF SPACE GROUP                             LEASTSQ   439
      IF(CENZON(H).EQ.0.)GO TO 20                                       LEASTSQ01  10
      ADCALC=(2.0*(FPB*REAL(M)-FPA*EMAG(M)))/(F(   MCPD)/QT   )         LEASTSQ   442
      E=ERR(   MCPD)/QT                                                 LEASTSQ   443
      ADOBS=AD(   MCPD)/QT                                              LEASTSQ   444
      IF(ADOBS.EQ.0.0) GO TO 20                                         LEASTSQ   445
      WT=1.0/(E*E)                                                      LEASTSQ   446
      ADDIF=ADOBS-ADCALC*CAY(M)                                         LEASTSQ   447
      ECALC(M,5,NORDER)=ECALC(M,5,NORDER)+ADDIF*ADDIF*WT                LEASTSQ   448
      ECALC(M,6,NORDER)=ECALC(M,6,NORDER)+ADOBS*ADCALC*WT               LEASTSQ   449
      ECALC(M,7,NORDER)=ECALC(M,7,NORDER)+ADCALC*ADCALC*WT              LEASTSQ   450
      ECALC(M,8,NORDER)=ECALC(M,8,NORDER)+WT                            LEASTSQ   451
 20   FSIZE(NS,1)=FSIZE(NS,1)+EPSQ                                      LEASTSQ   452
      FSIZE(NS,2)=FSIZE(NS,2)+1.0                                       LEASTSQ   453
  459 NV1=0                                                             LEASTSQ   454
      N=NCRYST(M)                                                       LEASTSQ   455
      DO 440 K=1,N                                                      LEASTSQ   456
      IF(K1.EQ.K) NV1=NV                                                LEASTSQ   457
  440 NV=NV+1+IFBOVR(M,K)                                               LEASTSQ   458
      IF(K1.EQ.0) GO TO 59                                              LEASTSQ   459
      DERIV(NV1) =DF/Q(M,K1)                                            LEASTSQ   460
      IF(IFBOVR(M,K1).EQ.0) GO TO 59                                    LEASTSQ   461
      NV1=NV1+1                                                         LEASTSQ   462
      DERIV(NV1)=DF*DSTSQ*0.25                                          LEASTSQ   463
   59 CONTINUE                                                          LEASTSQ   464
      N=NATOM(M)                                                        LEASTSQ   465
C                                                                       LEASTSQ   466
C G CALCULATE DERIVATIVES ON ATOMIC NUMBER, X# Y# Z# TEMP. FACTOR       LEASTSQ   467
C                                                                       LEASTSQ   468
      DO 37 K=1,N                                                       LEASTSQ   469
      ISF=NTROP(L)                                                      LEASTSQ   470
      IF(KK1(M).NE.0) GO TO 58                                          LEASTSQ   471
      DO 66 KK=2,4                                                      LEASTSQ   472
 66   NV=NV+LABEL(L,KK)                                                 LEASTSQ   473
      NV=NV+LABEL(L,1)*NCRYST(M)                                        LEASTSQ   474
      NV=NV+LABEL(L,5)*ISF                                              LEASTSQ   475
      GO TO 48                                                          LEASTSQ   476
 58   IF(LABEL(L,1).EQ.0) GO TO 67                                      LEASTSQ   477
      K1=KK1(M)                                                         LEASTSQ   478
      NV1=NV+K1-1                                                       LEASTSQ   479
      DERIV(NV1)=AXCON*DDANUM(L,K1,1)+BYCON*DDANUM(L,K1,2)              LEASTSQ   480
      NV=NV+NCRYST(M)                                                   LEASTSQ   481
 67   IF(LABEL(L,2).EQ.0) GO TO 68                                      LEASTSQ   482
      DERIV(NV)=AXCON*DDX(L,1)+BYCON*DDX(L,2)                           LEASTSQ   483
      NV=NV+1                                                           LEASTSQ   484
 68   IF(LABEL(L,3).EQ.0) GO TO 69                                      LEASTSQ   485
      DERIV(NV)=AXCON*DDY(L,1)+BYCON*DDY(L,2)                           LEASTSQ   486
      NV=NV+1                                                           LEASTSQ   487
 69   IF(LABEL(L,4).EQ.0) GO TO 70                                      LEASTSQ   488
      DERIV(NV)=AXCON*DDZ(L,1)+BYCON*DDZ(L,2)                           LEASTSQ   489
      NV=NV+1                                                           LEASTSQ   490
 70   IF(LABEL(L,5).EQ.0) GO TO 48                                      LEASTSQ   491
      DO 36 IS=1,ISF                                                    LEASTSQ   492
      DERIV(NV)=AXCON*DDB(L,IS,1)+BYCON*DDB(L,IS,2)                     LEASTSQ   493
 36   NV=NV+1                                                           LEASTSQ   494
 48   L=L+1                                                             LEASTSQ   495
```

$$ADCALC = \frac{2.0 * (B_P\ A_{HA} - A_P\ B_{HA})}{(\frac{SCL}{SHAPE}) * F_{PH}}$$

$$E = (\frac{SCL}{SHAPE}) * ERR(i) = (\frac{SCL}{SHAPE}) * \sigma F_{PH}$$

$$ADOBS = (\frac{SCL}{SHAPE}) * AD$$

$$WT = 1/(E)^2$$

ADDIF = ADOBS − (ADCALC*CAY)

NV1 = 0

DERIV(1) depending on whether BOVER refined

= SHAPE * FPHcalc to refine SCL

$$DERIV(_{BOVER}) = (\frac{SHAPE}{SCL} * F_{PHcalc} * \frac{\sin^2\theta}{\lambda^2})$$

d_1 for SCL

d_2 for BOVER

d_3 for ANUM atom 1

d_4 for x atom 1

d_5 for y atom 1

d_6 for z atom 1

d_7 for B atom 1

d_8 for ANUM atom 2

$$DERIV(_{ANUM}) = \cos\alpha_{PHcalc} * DDANUM(L,K1,1) + \sin\alpha_{PHcalc} * DDANUM(L,K1,2)$$

$$DERIV(_X) = \cos\alpha_{PHcalc} * DDX(L,1) + \sin\alpha_{PHcalc} * DDX(L,2)$$

similarly for Y and Z

$$DERIV(_B) = \cos\alpha_{PHcalc} * DDB(L,IS,1) + \sin\alpha_{PHcalc} * DDB(L,IS,2)$$

matrix m x n

m = n = # variables

NZ = flag for particular HA deriv

KK1 designates crystal of a given HA derivative

```
 37    CONTINUE
       DO 39 MM=1,NVAR
       DO 40 NN=1,NVAR
 40    TRIX(MM,NN)=TRIX(MM,NN)+DERIV(MM)*DERIV(NN)*W
 39    RHS(MM)=RHS(MM)+DERIV(MM)*EPSILN*W
 34    CONTINUE
 16    CONTINUE
C
C G END
C F END
C
C GO BACK TO READ IN NEW BLOCK OF DATA
       GO TO 15
C
C      END OF EACH CYCLE
   89  CONTINUE
       DO 71 M=1,NVAR
       CORLAT(M)=TRIX(M,M)
       DO 72 N=1,NVAR
 72    TRIX(M,N)=TRIX(M,N)/CORLAT(M)
 71    RHS(M)=RHS(M)/CORLAT(M)
       IF(CORLAT(M).EQ.0) WRITE(IW,530) M,N
530    FORMAT("0ZERO CORLAT" ,2I5)
       CALL MATINV(TRIX,NVAR,RHS,1,DETERM)
       DO 73 M=1,NVAR
       DO 73 N=1,NVAR
 73    TRIX(N,M)=TRIX(N,M)/CORLAT(M)
       WRITE(IW,97)TITLE
       WRITE(IW,95)
       DO 51 M=1,NVAR
       DO 52 N=1,NVAR
       CORLAT(N)=0.0
       IF(N.LT.M) GO TO 52
       CORLAT(N)=TRIX(M,N)/SQRT(TRIX(M,M)*TRIX(N,N))
 52    CONTINUE
 51    PRINT 94,  (CORLAT(N),N=1,NVAR)
       CALL FINAL(NVAR,NCPDS,MARK)
 50    CONTINUE
C
C B END
C C END
C
       IH=999
       IK=999
       IL=999
       FBEST=-1.0
       IF( IOUT.EQ.0.OR.IOUT.EQ.IP)GO TO 49
       WRITE(IOUT,60) IH,IK,IL,UNIT,UNIT,FBEST,UNIT,UNIT,UNIT
 49    IF(FIGMIN.EQ.0.0) GO TO 44
       H1=1000.0
       WRITE(ITT) H1,H2,H3,FP,A1,A2,((R(I,J),I=1,4),J=1,NCPDS)
       REWIND ITT
   44  IF( IOUT.EQ.0.OR.IOUT.EQ.IP)STOP
       END FILE IOUT
       REWIND IOUT
       STOP
       END
       SUBROUTINE CONRCP(AREAL,ARECIP)
       DIMENSION AREAL(6),ARECIP(6)
       RADC=3.1415926536/180.
       DO 100 I=1,3
       IF(AREAL(I+3).GT.1.)AREAL(I+3)=COS(AREAL(I+3)*RADC)
```

Matrix

$a_{ij} = \Sigma w d_i d_j$

$r_i = \Sigma d_i (W*EPSILN)$

$c_m = a_{mm}$ = diagonal

$a'_{m,n} = a_{mn}/c_m$

$r_m = r_m/c_m$

List if $c_m = 0$

Call MATINV A = TRIX a'_{ij}

N = NVAR i_{max}

$a' \rightarrow a''$ B = RHS b_i

M = 1

DETERM

$a'''_{nm} = a''_{nm}/c_m$

$c_n' = a'''_{mn} / \sqrt{a'''_{mm} * a'''_{nn}}$

Print out c_n'

Write statements

SUBROUTINE CONRCP

If $a,b,c,\alpha,\beta,\gamma \rightarrow a,b,c,\cos\alpha,\cos\beta,\cos\gamma$

$V = (abc \sqrt{1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma})$

$a^* = bc\sin\alpha/V$ etc.

$\cos\alpha^* = \dfrac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$ etc.

```
100   CONTINUE                                                          LEASTSQ02  10
      V=1.+2.*AREAL(4)*AREAL(5)*AREAL(6)-AREAL(4)**2-AREAL(5)**2-AREAL(6 LEASTSQ02  11
     * )**2                                                             LEASTSQ02  12
      V=AREAL(1)*AREAL(2)*AREAL(3)*SQRT(V)                              LEASTSQ02  13
      ASTAR=AREAL(2)*AREAL(3)*SQRT(1.-AREAL(4)**2)/V                    LEASTSQ02  14
      BSTAR=AREAL(3)*AREAL(1)*SQRT(1.-AREAL(5)**2)/V                    LEASTSQ02  15
      CSTAR=AREAL(1)*AREAL(2)*SQRT(1.-AREAL(6)**2)/V                    LEASTSQ02  16   This subroutine is called if real cell dimensions are given
      CAS=(AREAL(5)*AREAL(6)-AREAL(4))/(SQRT(1.-AREAL(5)**2)*SQRT(1.-ARE LEASTSQ02  17
     * AL(6)**2))                                                       LEASTSQ02  18
      CBS=(AREAL(6)*AREAL(4)-AREAL(5))/(SQRT(1.-AREAL(6)**2)*SQRT(1.-ARE LEASTSQ02  19
     * AL(4)**2))                                                       LEASTSQ02  20
      CCS=(AREAL(4)*AREAL(5)-AREAL(6))/(SQRT(1.-AREAL(4)**2)*SQRT(1.-ARE LEASTSQ02  21
     * AL(5)**2))                                                       LEASTSQ02  22
      ARECIP(4)=2.*ASTAR*BSTAR*CCS                                      LEASTSQ02  23
      ARECIP(5)=2.*BSTAR*CSTAR*CAS                                      LEASTSQ02  24
      ARECIP(6)=2.*CSTAR*ASTAR*CBS                                      LEASTSQ02  25
      ARECIP(1)=ASTAR**2                                                LEASTSQ02  26
      ARECIP(2)=BSTAR**2                                                LEASTSQ02  27
      ARECIP(3)=CSTAR**2                                                LEASTSQ02  28
      RETURN                                                            LEASTSQ02  29
      END                                                               LEASTSQ02  30
      FUNCTION CENZON(H)                                                LEASTSQ01  12       FUNCTION CENZON
      DIMENSION H(3)                                                    LEASTSQ01  13
      CENZON=H(1)*H(2)*H(3)                                             LEASTSQ01  14   hkℓ (used to check centric zone)
      RETURN                                                            LEASTSQ01  15   change this with space group
      END                                                               LEASTSQ01  16
      SUBROUTINE IOSET                                                  LEASTSQ   555
      COMMON /DEVICE/ IIN, IOUT, INCARD, FMT(20),IOUT1,IOUT2,           LEASTSQ   556       SUBROUTINE IOSET
     1 IOUT3,IOUT4,MMM,IM,IW,IP,ITT                                     LEASTSQ   557
      DIMENSION AF(8), AAD(8),AERR(8),AAA(20)                           LEASTSQ   558   Determines how  input and output handled
      DIMENSION NNHV(8)                                                 LEASTSQ05   7   Card read in to control this
C                                                                       LEASTSQ01  17
C     BNL I/O, ADAPTED FROM DUKE I/O ADAPTED FROM PURDUE                LEASTSQ01  18
C                                                                       LEASTSQ01  19
      IM=5                                                              LEASTSQ01  20
      IW=6                                                              LEASTSQ01  21
      IP=7                                                              LEASTSQ01  22
      ITT=20                                                            LEASTSQ01  23
      READ(IM,10)IIN,IOUT,INCARD,IOUT1,IOUT2,IOUT3,IOUT4,MMM            LEASTSQ   564
   10 FORMAT(8I5)                                                       LEASTSQ   565
      IOUT2=2                                                           LEASTSQ01  24
      IIN=14                                                            LEASTSQ01  25
      IF(INCARD.NE.0)IIN=2                                              LEASTSQ01  26
      IF(IOUT1.NE.0)IOUT1=1                                             LEASTSQ01  27
      IF(IOUT3.NE.0)IOUT3=3                                             LEASTSQ01  28
      IF(IOUT4.NE.0)IOUT4=4                                             LEASTSQ01  29
      IF(IOUT.NE.0)IOUT=IP                                              LEASTSQ01  30
      IF(INCARD.EQ.0) RETURN                                            LEASTSQ   566
      REWIND IIN                                                        LEASTSQ05   8
100   CALL CARDIN(IM ,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP,  LEASTSQ05   9
     * FIGMER,NNHV,AF,AERR,AAD)                                         LEASTSQ05  10
      CALL TAPOUT(IIN,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP,  LEASTSQ05  11
     * FIGMER,NNHV,AF,AERR,AAD)                                         LEASTSQ05  12
      IF(NNO.GT.0)GO TO 100                                             LEASTSQ05  13
      ENDFILE IIN                                                       LEASTSQ05  14
      REWIND IIN                                                        LEASTSQ05  15
      RETURN                                                            LEASTSQ   583       SUBROUTINE TAPEIN
      END                                                               LEASTSQ   584
      SUBROUTINE TAPEIN(IIN,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,  LEASTSQ05  16   Reading of tape
     * FAZMP,FIGMER,NNHV,F,ERR,AD)                                      LEASTSQ05   1
      DIMENSION NNHV(8),F(8),ERR(8),AD(8)                               LEASTSQ05   1       If EOF is met, put NNO to 0
100   READ(IIN)NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP,FIGMER,  LEASTSQ05   1       MODIFY is called
```

```
     * (NNHV(II),F(II),ERR(II),AD(II),II=1,8)                          LEASTSQ05  20
      IF(EOF(IIN))105,1105                                              LEASTSQ05  21
 105  NNO=0                                                             LEASTSQ05  22
 1105 CALL MODIFY(IIN,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP,  LEASTSQ05  23
     * FIGMER,NNHV,F,ERR,AD)                                            LEASTSQ05  24
      IF(NNO.LT.0)GO TO 100                                             LEASTSQ05  25
      RETURN                                                            LEASTSQ05  26
      END                                                               LEASTSQ05  27
      SUBROUTINE CARDIN(IM,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,   LEASTSQ05  28
     * FAZMP,FIGMER,NNHV,F,ERR,AD)                                      LEASTSQ05  29
      DIMENSION NNHV(8),F(8),ERR(8),AD(8)                               LEASTSQ05  30
      DATA NN/0/                                                        LEASTSQ05  31
 100  FORMAT(3I3,2F6.2,I2,2X,3F6.2,I2,2X,3F6.2,I2)                      LEASTSQ05  32
      IF(NN.GT.0)GO TO 200                                              LEASTSQ05  33
      DO 10 I=1,8                                                       LEASTSQ05  34
      NNHV(I)=0                                                         LEASTSQ05  35
      F(I)=0.                                                           LEASTSQ05  36
      ERR(I)=.1                                                         LEASTSQ05  37
      AD(I)=0                                                           LEASTSQ05  38
 10   CONTINUE                                                          LEASTSQ05  39
      ADNAT=0.                                                          LEASTSQ05  40
      FAZBST=0                                                          LEASTSQ05  41
      FAZMP=0.                                                          LEASTSQ05  42
      FIGMER=.1                                                         LEASTSQ05  43
 200  READ(IM,100)IH,IK,IL,FNAT,ERNAT,NNAT,(F(II),AD(II),ERR(II),NNHV(II LEASTSQ05  44
     * ),II=1,2)                                                        LEASTSQ05  45
      NN=NN+1                                                           LEASTSQ05  46
      NNO=NN                                                            LEASTSQ05  47
      IF(IABS(IH)+IABS(IK)+IABS(IL).EQ.0)NNO=0                          LEASTSQ05  48
      NNAT=1-NNAT                                                       LEASTSQ05  49
      NNHV(1)=1-NNHV(1)                                                 LEASTSQ05  50
      NNHV(2)=1-NNHV(2)                                                 LEASTSQ05  51
      RETURN                                                            LEASTSQ05  52
      END                                                               LEASTSQ05  53
      SUBROUTINE TAPOUT(IOUT,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,        LEASTSQ05  54
     * FAZBST,FAZMP,FIGMER,NNHV,F,ERR,AD)                               LEASTSQ05  55
      DIMENSION NNHV(8),F(8),ERR(8),AD(8)                               LEASTSQ05  56
      WRITE(IOUT)NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,FAZMP,       LEASTSQ05  57
     * FIGMER,((NNHV(II),F(II),ERR(II),AD(II)),II=1,8)                  LEASTSQ05  58
      RETURN                                                            LEASTSQ05  59
      END                                                               LEASTSQ05  60
      SUBROUTINE MODIFY(IIN,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT,FAZBST,  LEASTSQ05  61
     * FAZMP,FIGMER,NNHV,F,ERR,AD)                                      LEASTSQ05  62
      DIMENSION NNHV(8),F(8),ERR(8),AD(8)                               LEASTSQ05  63
      RETURN                                                            LEASTSQ05  64
      END                                                               LEASTSQ05  65
      SUBROUTINE PHASE(I,ALPHA,SCALE,NCPDS,IANGLE,CAY,FIGMIN,           LEASTSQ    585
     1 UNIT,IFPRNT,NORDER,MARK,Q,DSTSQ,BOVER,KK1)                       LEASTSQ    586
      COMMON /DEVICE/ IIN, IOUT, INCARD, FMT(20),IOUT1,IOUT2,           LEASTSQ    587
     1 IOUT3,IOUT4,MMM,IM,IW,IP,ITT                                     LEASTSQ    588
      COMMON STAB(450),ETAB(450),NFS(8),RVAL(8,9,9),RCEN(8,9,9),        LEASTSQ    589
     1 TITLE(20),EIS(8,9),EAD(8,9),FSIZE(8,3),FIG(2,9),DSTRB(10),GAP    LEASTSQ    590
      COMMON/DATA/H(3),FNAT,F(8),ERR(8),AD(8),ERNAT,ADNAT,NNO,NNAT,     LEASTSQ    591
     1 NNHV(8),FAZBST,FAZMP,FIGMER,REAL(8),EMAG(8)                      LEASTSQ    592
      DIMENSION CAY(8),PHI(8),P(360),X(8,2),OUT(9),ALPH(9),Q(8,10)      LEASTSQ    593
      DIMENSION FH(8,4)                                                 LEASTSQ    594
      DIMENSION BOVER(8,10)  ,KK1(8)                                    LEASTSQ    595
      INTEGER PHI                                                       LEASTSQ    596
C                                                                       LEASTSQ    597
C A COLLECT INFORMATION# FH(OBS), H(CALC), DELTA(FH)OBS, ETC            LEASTSQ    598
C                                                                       LEASTSQ    599
      KOUNT=0                                                           LEASTSQ    600
```

SUBROUTINE CARDIN

Subroutine for cards in the format we had it

0 for obs 1 for unobs etc.

h k ℓ F_P σF_P 0 or 1 F_{PH}

AD_{PH} σ_{PH} 0 or 1 etc.

SUBROUTINE TAPOUT

Tape out

Write hkℓ etc on tape

SUBROUTINE MODIFY

This can be changed as required

SUBROUTINE PHASE

QT = SHAPE/SCL

FP = SCALE * FNAT

$FH(M,1) = (\frac{SCL}{SHAPE}) * FPH = F_{PHcorr}$

$FH(M,2) = f_{HA}$ = SMALLF

= structure factor for heavy atom alone

```
      IF(FNAT    .GT.0.0) KOUNT=1                                  LEASTSQ   601
      FP=FNAT    *SCALE                                            LEASTSQ   602
      DO 10 M=1,NCPDS                                              LEASTSQ   603
      MCPD=NFS(M)                                                  LEASTSQ   604
      FH(M,1)=0.0                                                  LEASTSQ   605
      FH(M,2)=0.0                                                  LEASTSQ   606
      FH(M,3)=0.0                                                  LEASTSQ   607
      IF(KK1(M).EQ.0) GO TO 10                                     LEASTSQ   608
      K1=KK1(M)                                                    LEASTSQ   609
      QT=Q(M,K1)*EXP(BOVER(M,K1)*DSTSQ*0.25)                       LEASTSQ   610
C TO AVOID ZERO ARGUMENTS IN ATAN2 FUNCTION                        LEASTSQ   611
      IF(EMAG(M).EQ.0.0.AND.REAL(M).EQ.0.0) GO TO 10               LEASTSQ   612
       IF(EMAG(M).EQ.0.0) EMAG(M) = 1.0E-10                        LEASTSQ   613
       IF(REAL(M).EQ.0.0) REAL(M) = 1.0E-10                        LEASTSQ   614
      KOUNT=KOUNT+1                                                LEASTSQ   615
      FH(M,1)=F(  MCPD)/QT                                         LEASTSQ   616
      FH(M,2)=SQRT(REAL(M)*REAL(M)+EMAG(M)*EMAG(M))                LEASTSQ   617
      PHI(M)=IFIX(((ATAN2(EMAG(M),REAL(M))+6.2832)*57.296)+0.5)    LEASTSQ   618
      IF(CAY(M).EQ.0.0) GO TO 10                                   LEASTSQ   619
      E=ERR(  MCPD)/QT                                             LEASTSQ   620
      FH(M,3)=AD(  MCPD)/QT                                        LEASTSQ   621
      RATIO=EAD(M,NORDER)/75.0                                     LEASTSQ   622
      IF(RATIO.LT.0.33) RATIO=0.33                                 LEASTSQ   623
      IF(RATIO.GT.3.00) RATIO=3.00                                 LEASTSQ   624
      IF(EAD(M,NORDER).EQ.0.0) RATIO=1.0                           LEASTSQ   625
      FH(M,4)=E*RATIO                                              LEASTSQ   626
   10 CONTINUE                                                     LEASTSQ   627
C                                                                  LEASTSQ   628
C A END                                                            LEASTSQ   629
C                                                                  LEASTSQ   630
  200 CONTINUE                                                     LEASTSQ   631
      IF( KOUNT.GE.2) GO TO 40                                     LEASTSQ   632
      ALPHA=-10.0                                                  LEASTSQ   633
      GO TO 24                                                     LEASTSQ   634
C                                                                  LEASTSQ   635
C     ALPHA INCREMENT                                              LEASTSQ   636
 40   C=0.0                                                        LEASTSQ   637
      D=0.0                                                        LEASTSQ   638
      SUM=0.0                                                      LEASTSQ   639
      PMAX=0.0                                                     LEASTSQ   640
      INC=IANGLE                                                   LEASTSQ   641
C                                                                  LEASTSQ   642
C B CALC PROBABILITY FOR PROTEIN PHASES FOR SERIES OF ANGLES       LEASTSQ   643
C      BEST PHASE, ANGLES FIGURE OF MERITS                         LEASTSQ   644
C                                                                  LEASTSQ   645
      IF(CENZON(H).EQ.0.) INC=180                                  LEASTSQ01  46
      ISTART=1                                                     LEASTSQ   648
      DO 11 J=ISTART,360,INC                                       LEASTSQ   649
      P(J)=1.0                                                     LEASTSQ   650
      JANGLE=J-1                                                   LEASTSQ   651
      JTRUE=JANGLE+180                                             LEASTSQ   652
C                                                                  LEASTSQ   653
C     INTERSECTION OF CIRCLES WITH RADIUS VECTOR                   LEASTSQ   654
      DO 13 M=1,NCPDS                                              LEASTSQ   655
      MCPD=NFS(M)                                                  LEASTSQ   656
      IF(KK1(M).EQ.0) GO TO 13                                     LEASTSQ   657
      IAPHI=JANGLE-PHI(M)                                          LEASTSQ   658
 44   IF(IAPHI.GT.0) GO TO 43                                      LEASTSQ   659
      IAPHI=IAPHI+360                                              LEASTSQ   660
      GO TO 44                                                     LEASTSQ   661
 43   IF(IAPHI.LE.360) GO TO 45                                    LEASTSQ   662
      IAPHI=IAPHI-360                                              LEASTSQ   663
```

$FH(M,3) = (\frac{SCL}{SHAPE}) * (F^{+}-F^{-})$

$PHI(M) = \alpha_{HA} = \alpha_j$ = phase angle for heavy atom

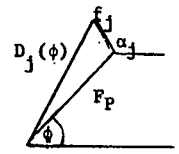
$E = (\frac{SCL}{SHAPE}) * \sigma F$

$FH(M,4) = (\frac{SCL}{SHAPE}) * \frac{\sigma F_{PH} * EAD}{75}$

$= E_j/75$

For isomorphism

JTRUE = ϕ under consideration



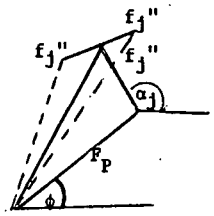
$$D_j(\phi) = \sqrt{F_P^{\,2} + f_j^{\,2} + 2F_P f_j \cos(\phi-\alpha_j)}$$

$= X(M,1)$

For anomalous dispersion

$D_{anom}(\phi) = 2(F_P f_j''/D_{j(\phi)})\sin(\phi-\alpha_j)$

$= X(M,2)$



$DIFIS = F_{PHcorr} - D_j(\phi)$

$= F_{PHcorr} - F_{PHisomcalc} = FH(M,1) - X(M,1)$

$DIFABS = \epsilon_j(\phi) = |F_{PHcorr} - F_{PHisomcalc}| = ABS(DIFIS)$

```
      GO TO 43                                                          LEASTSQ   664
C CALCULATE FHP                                                         LEASTSQ   665
 45   X(M,1)=SQRT(FP*FP+FH(M,2)*FH(M,2)-2.0*FP*FH(M,2)*STAB(IAPHI+90))  LEASTSQ   666
 14   IF(CAY(M).EQ.0.0) GO TO 13                                        LEASTSQ   667
      ITPHI=JTRUE-PHI(M)                                                LEASTSQ   668
 46   IF(ITPHI.GT.0) GO TO 47                                           LEASTSQ   669
      ITPHI=ITPHI+360                                                   LEASTSQ   670
      GO TO 46                                                          LEASTSQ   671
 47   IF(ITPHI.LE.360) GO TO 48                                         LEASTSQ   672
      ITPHI=ITPHI-360                                                   LEASTSQ   673
      GO TO 47                                                          LEASTSQ   674
C CALCULATE ANORMALOUS DIFFERENCES                                      LEASTSQ   675
 48   X(M,2)=(2.0*FP*CAY(M)*FH(M,2)*STAB(ITPHI))/X(M,1)                 LEASTSQ   676
  13  CONTINUE                                                          LEASTSQ   677
C                                                                       LEASTSQ   678
C     FIND MEAN OF ALL INTERSECTIONS                                    LEASTSQ   679
C                                                                       LEASTSQ   680
C     PHASE PROBABILITY FOR GIVEN INTERSECTIONS                         LEASTSQ   681
  15  DO 16 M=1,NCPDS                                                   LEASTSQ   682
      MCPD=NFS(M)                                                       LEASTSQ   683
      IF(KK1(M).EQ.0) GO TO 18                                          LEASTSQ   684
      DIFIS=FH(M,1)-X(M,1)                                              LEASTSQ   685
      DIFABS=ABS(DIFIS)                                                 LEASTSQ   686
      IEXPO=IFIX((DIFABS*150.0)/EIS(M,NORDER))+1                        LEASTSQ   687
      IF(IEXPO.GT.450) IEXPO=450                                        LEASTSQ   688
      P(J)=P(J)*ETAB(IEXPO)                                             LEASTSQ   689
 18   IF((CAY(M).EQ.0.0).OR.(FP.EQ.0.0).OR.(INC.EQ.180).OR.             LEASTSQ   690
     1(FH(M,4).EQ.0.0).OR.(FH(M,3).EQ.0.0)) GO TO 16                    LEASTSQ   691
      DIFAD=FH(M,3)-X(M,2)                                              LEASTSQ   692
      DIFABS=ABS(DIFAD)                                                 LEASTSQ   693
      IEXPO=IFIX((DIFABS*150.0)/FH(M,4))+1                              LEASTSQ   694
      IF(IEXPO.GT.450) IEXPO=450                                        LEASTSQ   695
      P(J)=P(J)*ETAB(IEXPO)                                             LEASTSQ   696
  16  CONTINUE                                                          LEASTSQ   697
      IF(JTRUE.LE.360) GO TO 49                                         LEASTSQ   698
      JTRUE=JTRUE-360                                                   LEASTSQ   699
 49   C=C+P(J)*STAB(JTRUE+90)                                           LEASTSQ   700
      D=D+P(J)*STAB(JTRUE)                                              LEASTSQ   701
      SUM=SUM+P(J)                                                      LEASTSQ   702
C                                                                       LEASTSQ   703
C     FIND MOST PROBABLE PHASE AND STORE CORRESPONDING ERRORS           LEASTSQ   704
      IF(P(J).LT.PMAX) GO TO 11                                         LEASTSQ   705
      AMAX=FLOAT(JTRUE)                                                 LEASTSQ   706
      PMAX=P(J)                                                         LEASTSQ   707
  11  CONTINUE                                                          LEASTSQ   708
C                                                                       LEASTSQ   709
C B END                                                                 LEASTSQ   710
C                                                                       LEASTSQ   711
C     DETERMINE FBEST,ABEST,FIG OF MERIT AND SUM ERROR CONTRIBUTIONS    LEASTSQ   712
 37   FBEST=SQRT(C*C+D*D)/SUM                                           LEASTSQ   713
C TO AVOID ZERO ARGUMENTS IN ATAN2 FUNCTION                             LEASTSQ   714
      IF( C.EQ.0.0.AND.D.EQ.0.0) GO TO 200                              LEASTSQ   715
      IF(C.EQ.0.0) C=1.0E-10                                            LEASTSQ   716
      IF(D.EQ.0.0) D=1.0E-10                                            LEASTSQ   717
      ABEST=ATAN2(D,C)                                                  LEASTSQ   718
      IF(ABEST.LT.0.0) ABEST=ABEST+6.2832                               LEASTSQ   719
      AMAX=AMAX*0.017453                                                LEASTSQ   720
      FIG(1,NORDER)=FIG(1,NORDER)+FBEST                                 LEASTSQ   721
      FIG(2,NORDER)=FIG(2,NORDER)+1.0                                   LEASTSQ   722
      FIG(1,9)=FIG(1,9)+FBEST                                           LEASTSQ   723
      FIG(2,9)=FIG(2,9)+1.0                                             LEASTSQ   724
      IJ=1+IFIX(FBEST/0.1)                                              LEASTSQ   725
```

$$P(J) = P(\phi) = \prod \exp\left\{-\frac{\Sigma(\varepsilon_j(\phi))^2}{2E_j^{\,2}}\right\}$$

$$DIFAD = AD_{corr} - AD_{anomcalc} = \varepsilon'(\phi) = FH(M,3) - X(M,2)$$

$$DIFABS = ABS(DIFAD)$$

$$P = P(\phi) * P(\phi)_{anom}$$

$$P(\phi)_{anom} = \prod \exp\left\{-\frac{(\varepsilon')^2}{2E_j^{\,2}}\right\}$$

$$\text{Figure of merit} = \bar{m} = FBEST = (\sqrt{C^2 + D^2})/SUM$$

$$C = \Sigma P(\phi)\cos\phi$$

$$D = \Sigma P(\phi)\sin\phi$$

$$SUM = \Sigma P(\phi)$$

$$ABEST = \phi_{best} = \text{best phase} = \tan^{-1}(D/C)$$

$$AMAX = \phi_{max} = \text{most probable phase}$$

```
      IF(IJ.GT.10) IJ=10                                                LEASTSQ   726
      DSTRB(IJ)=DSTRB(IJ)+1.0                                           LEASTSQ   727
      ALPHA=AMAX                                                        LEASTSQ   728
C                                                                       LEASTSQ   729
C     PRODUCE DESIRED PHASE OUTPUT                                      LEASTSQ   730
      IH=H(1)                                                           LEASTSQ   731
      IK=H(2)                                                           LEASTSQ   732
      IL=H(3)                                                           LEASTSQ   733
      IF(IOUT1.NE.0)CALL TAPOUT(IOUT1,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT LEASTSQ005  66
     * ,ABEST,AMAX,FBEST,NNHV,F,ERR,AD)                                 LEASTSQ005  67
 23   IF(MARK.NE.0) GO TO 24                                            LEASTSQ   736
      X(1,1)=FP*COS(ABEST)                                              LEASTSQ   737
      Y=FP*SIN(ABEST)                                                   LEASTSQ   738
      OUT(1)=FP                                                         LEASTSQ   739
      ALPH(1)=ABEST*57.294                                              LEASTSQ   740
      DO 20 J1=2,9                                                      LEASTSQ   741
      OUT(J1)=0.0                                                       LEASTSQ   742
 20   ALPH(J1)=0.0                                                      LEASTSQ   743
      DST=SQRT(DSTSQ)                                                   LEASTSQ   744
      DO 21 M=1,NCPDS                                                   LEASTSQ   745
      MCPD=NFS(M)                                                       LEASTSQ   746
      IF(KK1(M).EQ.0) GO TO 21                                          LEASTSQ   747
      K1=KK1(M)                                                         LEASTSQ   748
      QT=Q(M,K1)*EXP(BOVER(M,K1)*DSTSQ*0.25)                            LEASTSQ   749
      J=M+1                                                             LEASTSQ   750
      AA=X(1,1)+REAL(M)                                                 LEASTSQ   751
      BB=Y+EMAG(M)                                                      LEASTSQ   752
C TO AVOID ZERO ARGUMENTS IN ATAN2 FUNCTION                             LEASTSQ   753
      IF(BB.EQ.0.0.AND.AA.EQ.0.0) GO TO 200                             LEASTSQ   754
      AH=ATAN2(BB,AA)                                                   LEASTSQ   755
      AX1=F(MCPD)*COS(AH)/QT                                            LEASTSQ   756
      AY1=F(MCPD)*SIN(AH)/QT                                            LEASTSQ   757
      AX2= X(1,1) + REAL(M)                                             LEASTSQ   758
      AY2 = Y + EMAG(M)                                                 LEASTSQ   759
      AX=AX1-AX2                                                        LEASTSQ   760
      AY=AY1-AY2                                                        LEASTSQ   761
      IF(MMM.EQ.M.AND.IOUT4.NE.0) WRITE(IOUT4) IH,IK,IL,DST,AX1,AX2,    LEASTSQ   762
     1 AY1,AY2                                                          LEASTSQ   763
      OUT(J)=SQRT(AX*AX+AY*AY)                                          LEASTSQ   764
      ALPH(J)=ATAN2(AY,AX)                                              LEASTSQ   765
      IF(ALPH(J).LT.0.0) ALPH(J)=ALPH(J)+6.2832                         LEASTSQ   766
      ALPH(J)=ALPH(J)*57.294                                            LEASTSQ   767
      IF(INC.NE.180) GO TO 41                                           LEASTSQ   768
      DO 42 J2=1,9                                                      LEASTSQ   769
      KUT=ALPH(J2)/179.0                                                LEASTSQ   770
 42   ALPH(J2)=KUT*180                                                  LEASTSQ   771
 41   IF((CAY(M).EQ.0.0).OR.(INC.EQ.180).OR.(FH(M,4).EQ.0.0)            LEASTSQ   772
     1.OR.(FH(M,3).EQ.0.0))GO TO 21                                     LEASTSQ   773
      JAD=J+3                                                           LEASTSQ   774
      IF((JAD.LE.(NCPDS+1)).OR.(JAD.GT.9)) GO TO 21                     LEASTSQ   775
      ADWT=FH(M,3)/(FH(M,4)*FH(M,4))                                    LEASTSQ   776
      OUT(JAD)=ADWT                                                     LEASTSQ   777
      ALPH(JAD)=(ABEST+1.5708)*57.294                                   LEASTSQ   778
 21   CONTINUE                                                          LEASTSQ   779
      AAA=FP*COS(ABEST)                                                 LEASTSQ   780
      AAA1=AAA*FBEST                                                    LEASTSQ   781
      BBB=FP*SIN(ABEST)                                                 LEASTSQ   782
      BBB1=BBB*FBEST                                                    LEASTSQ   783
      IF(IOUT3.NE.0) WRITE(IOUT3) IH,IK,IL,DST,AAA,AAA1,BBB,BBB1        LEASTSQ   784
      IF(IOUT.NE.0)WRITE(IOUT,101)IH,IK,IL,FP,ABEST,AAA,BBB,AMAX,FBEST  LEASTSQ   785
 101  FORMAT(3I3, 1X, 7F9.3 )                                           LEASTSQ   786
     0IF(IFPRNT.EQ.1) PRINT 100,IH,IK,IL,FP,ABEST,AMAX,FBEST,((M,FH(M,1) LEASTSQ   787
```

$QT = (SHAPE/SCL)$

$X(1,1) = F_P \cos\phi_{best}$

$Y = F_P \sin\phi_{best}$

$OUT(1) = F_P$

$ALPH(1) = \phi_{best}$

$AA = F_P \cos\phi_{best} + A_{HA} = A_{PHisom}$

$BB = F_P \sin\phi_{best} + B_{HA} = B_{PHisom}$

$AH = \phi_{PHisom}$

$$AX = \left(\frac{F_{PHobs} * SCL * \cos\phi_{PHisom}}{SHAPE}\right) - (F_{P\cos\phi_{best}} + A_{HA})$$

$$\approx A_{PH_X} - A_{PH_Y}$$

$$AY = \left(\frac{F_{PHobs} * SCL * \sin\phi_{PHisom}}{SHAPE}\right) - (F_P \sin\phi_{best} + B_{HA})$$

$$\approx B_{PH_X} - B_{PH_Y}$$

$$OUT(J) = \sqrt{(AX)^2 + (AY)^2}$$

$$ALPH(J) = \tan^{-1}(AY/AX)$$

weight for anomalous dispersion

$$ADWT = \frac{(F^+ - F^-) * SHAPE * (75)^2}{SCL * (\sigma F_{PH})^2 * (EAD)^2}$$

$OUT(JAD) = ADWT$

$ALPH(JAD) = (\phi_{best} + \pi/2)$

```
      IF(IJ.GT.10) IJ=10                                                LEASTSQ   726
      DSTRB(IJ)=DSTPR(IJ)+1.0                                           LEASTSQ   727
      ALPHA=AMAX                                                        LEASTSQ   728
C                                                                       LEASTSQ   729
C     PRODUCE DESIRED PHASE OUTPUT                                      LEASTSQ   730
      IH=H(1)                                                           LEASTSQ   731
      IK=H(2)                                                           LEASTSQ   732
      IL=H(3)                                                           LEASTSQ   733
      IF(IOUT1.NE.0)CALL TAPOUT(IOUT1,NNO,IH,IK,IL,NNAT,FNAT,ERNAT,ADNAT LEASTSQ05  66
     * ,ABEST,AMAX,FBFST,NNHV,F,ERR,AD)                                 LEASTSQ05  67
 23   IF(MARK.NE.0) GO TO 24                                            LEASTSQ   736
      X(1,1)=FP*COS(ABFST)                                              LEASTSQ   737
      Y=FP*SIN(ABEST)                                                   LEASTSQ   738
      OUT(1)=FP                                                         LEASTSQ   739
      ALPH(1)=ABEST*57.294                                              LEASTSQ   740
      DO 20 J1=2,9                                                      LEASTSQ   741
      OUT(J1)=0.0                                                       LEASTSQ   742
 20   ALPH(J1)=0.0                                                      LEASTSQ   743
      DST=SQRT(DSTSQ)                                                   LEASTSQ   744
      DO 21 M=1,NCPDS                                                   LEASTSQ   745
      MCPD=NFS(M)                                                       LEASTSQ   746
      IF(KK1(M).EQ.0) GO TO 21                                          LEASTSQ   747
      K1=KK1(M)                                                         LEASTSQ   748
      QT=Q(M,K1)*EXP(BOVER(M,K1)*DSTSQ*0.25)                            LEASTSQ   749
      J=M+1                                                             LEASTSQ   750
      AA=X(1,1)+REAL(M)                                                 LEASTSQ   751
      BB=Y+EMAG(M)                                                      LEASTSQ   752
C TO AVOID ZERO ARGUMENTS IN ATAN2 FUNCTION                             LEASTSQ   753
      IF(BB.EQ.0.0.AND.AA.EQ.0.0) GO TO 200                             LEASTSQ   754
      AH=ATAN2(BB,AA)                                                   LEASTSQ   755
      AX1=F(MCPD)*COS(AH)/QT                                            LEASTSQ   756
      AY1=F(MCPD)*SIN(AH)/QT                                            LEASTSQ   757
      AX2= X(1,1) + REAL(M)                                             LEASTSQ   758
      AY2 = Y + EMAG(M)                                                 LEASTSQ   759
      AX=AX1-AX2                                                        LEASTSQ   760
      AY=AY1-AY2                                                        LEASTSQ   761
      IF(MMM.EQ.M.AND.IOUT4.NE.0) WRITE(IOUT4) IH,IK,IL,DST,AX1,AX2,    LEASTSQ   762
     1 AY1,AY2                                                          LEASTSQ   763
      OUT(J)=SQRT(AX*AX+AY*AY)                                          LEASTSQ   764
      ALPH(J)=ATAN2(AY,AX)                                              LEASTSQ   765
      IF(ALPH(J).LT.0.0) ALPH(J)=ALPH(J)+6.2832                         LEASTSQ   766
      ALPH(J)=ALPH(J)*57.294                                            LEASTSQ   767
      IF(INC.NE.180) GO TO 41                                           LEASTSQ   768
      DO 42 J2=1,9                                                      LEASTSQ   769
      KUT=ALPH(J2)/179.0                                                LEASTSQ   770
 42   ALPH(J2)=KUT*180                                                  LEASTSQ   771
 41   IF((CAY(M).EQ.0.0).OR.(INC.EQ.180).OR.(FH(M,4).EQ.0.0)            LEASTSQ   772
     1.OR.(FH(M,3).EQ.0.0))GO TO 21                                     LEASTSQ   773
      JAD=J+3                                                           LEASTSQ   774
      IF((JAD.LE.(NCPDS+1)).OR.(JAD.GT.9)) GO TO 21                     LEASTSQ   775
      ADWT=FH(M,3)/(FH(M,4)*FH(M,4))                                    LEASTSQ   776
      OUT(JAD)=ADWT                                                     LEASTSQ   777
      ALPH(JAD)=(ABEST+1.5708)*57.294                                   LEASTSQ   778
 21   CONTINUE                                                          LEASTSQ   779
      AAA=FP*COS(ABFST)                                                 LEASTSQ   780
      AAA1=AAA*FBEST                                                    LEASTSQ   781
      BBB=FP*SIN(ABEST)                                                 LEASTSQ   782
      BBB1=BBB*FBEST                                                    LEASTSQ   783
      IF(IOUT3.NE.0) WRITE(IOUT3) IH,IK,IL,DST,AAA,AAA1,BBB,BBB1        LEASTSQ   784
      IF(IOUT.NE.0)WRITE(IOUT,101)IH,IK,IL,FP,ABEST,AAA,BBB,AMAX,FBEST  LEASTSQ   785
 101  FORMAT(3I3, 1X, 7F9.3 )                                           LEASTSQ   786
     0IF(IFPRNT.EQ.1) PRINT 100,IH,IK,IL,FP,ABEST,AMAX,FBEST,((M,FH(M,1) LEASTSQ   787
```

$QT = (SHAPE/SCL)$

$X(1,1) = F_P \cos\phi_{best}$

$Y = F_P \sin\phi_{best}$

$OUT(1) = F_P$

$ALPH(1) = \phi_{best}$

$AA = F_P \cos\phi_{best} + A_{HA} = A_{PHisom}$

$BB = F_P \sin\phi_{best} + B_{HA} = B_{PHisom}$

$AH = \phi_{PHisom}$

$$AX = \left(\frac{F_{PHobs} * SCL * \cos\phi_{PHisom}}{SHAPE}\right) - (F_P \cos\phi_{best} + A_{HA})$$

$$\approx A_{PH_X} - A_{PH_Y}$$

$$AY = \left(\frac{F_{PHobs} * SCL * \sin\phi_{PHisom}}{SHAPE}\right) - (F_P \sin\phi_{best} + B_{HA})$$

$$\approx B_{PH_X} - B_{PH_Y}$$

$$OUT(J) = \sqrt{(AX)^2 + (AY)^2}$$

$$ALPH(J) = \tan^{-1}(AY/AX)$$

weight for anomalous dispersion

$$ADWT = \frac{(F^+ - F^-) * SHAPE * (75)^2}{SCL * (\sigma F_{PH})^2 * (EAD)^2}$$

$OUT(JAD) = ADWT$

$ALPH(JAD) = (\phi_{best} + \pi/2)$

```
     1,FH(M,3),FH(M,2),PHI(M),REAL(M),EMAG(M)),M=1,NCPDS)                LEASTSQ   788
 100 FORMAT(1X,3I3,F8.2,2F6.3,F4.2,4(2(I3,3F8.2,I5,2F6.1),/))            LEASTSQ   789
30   IF(FBEST.GT.FIGMIN) GO TO 24                                        LEASTSQ   790
     A1=ABEST*57.294                                                     LEASTSQ   791
     A2=AMAX *57.294                                                     LEASTSQ   792
  2  FORMAT(1H 3F4.0,11H  F NATIVE= F8.0,15H  FIG OF MERIT=F5.3,         LEASTSQ   793
    1 35H  BEST AND MOST PROBABLE PHASES ARE 2F5.0)                      LEASTSQ   794
     PRINT 2,  (H(  J),J=1,3),FP,FBEST,A1,A2                             LEASTSQ   795
  3  FORMAT(4H CPD,7X,2HFH,8X,2HAD,4X,6HFSMALL,7X,3HPHI,7X,1HA,8X,1HB)   LEASTSQ   796
     WRITE(IW,3)                                                         LEASTSQ   797
     DO 25 M=1,NCPDS                                                     LEASTSQ   798
     DEG=FLOAT(PHI(M))                                                   LEASTSQ   799
  4  FORMAT(1H I3,3F10.0,I9,2F10.0)                                      LEASTSQ   800
     PRINT 4,  M,FH(M,1),FH(M,3),FH(M,2),PHI(M),REAL(M),EMAG(M)          LEASTSQ   801
 25  CONTINUE                                                            LEASTSQ   802
     H1=H(1)                                                             LEASTSQ   803
     H2=H(2)                                                             LEASTSQ   804
     H3=H(3)                                                             LEASTSQ   805
     WRITE(ITT) H1,H2,H3,FP,A1,A2,FBEST,(FH(M,1),FH(M,3),REAL(M),        LEASTSQ   806
    1  EMAG(M), M=1,NCPDS)                                               LEASTSQ   807
     JJ=0                                                                LEASTSQ   808
     DO 26  J=ISTART,360,INC                                             LEASTSQ   809
     JJ=JJ+1                                                             LEASTSQ   810
26   P(JJ)=P(J)/PMAX                                                     LEASTSQ   811
     JJ2=(JJ/2)+1                                                        LEASTSQ   812
  5  FORMAT(30H TOTAL PHASE PROBABILITY CURVE )                          LEASTSQ   813
     WRITE(IW,5)                                                         LEASTSQ   814
  6  FORMAT(1H 19F6.2)                                                   LEASTSQ   815
     PRINT 6,  (P(J),J=1,JJ2)                                            LEASTSQ   816
     PRINT 6,  (P(J),J=JJ2,JJ),P(1)                                      LEASTSQ   817
24   RETURN                                                              LEASTSQ   818
     END                                                                 LEASTSQ   819
     SUBROUTINE FINAL(NVAR,NCPDS,MARK)                                   LEASTSQ   820
     COMMON STAB(450),FTAB(450),NFS(8),RVAL(8,9,9),RCEN(8,9,9),          LEASTSQ   821
    1 TITLE(20),EIS(8,9),EAD(8,9),FSIZE(8,3),FIG(2,9),DSTRB(10),GAP      LEASTSQ   822
     COMMON/ATOMS/Q(8,10),Q1(8,10),BOVER(8,10),BOVR1(8,10),              LEASTSQ   823
    1 IFBOVR(8,10),ANUM(50,10),ANUM1(50,10),X(50),X1(50),Y(50),Y1(50),   LEASTSQ   824
    2 Z(50),Z1(50),B(50,6),B1(50,6),NTROP(50),LABEL(50,5),               LEASTSQ   825
    3 AMAGS,AMAGBO,AMAGX,AMAGY,AMAGZ,AMAGB,AMAGA,CPDTLE(8,2),            LEASTSQ   826
    4 CAY(8),NATOM(8),NCRYST(8),KK1(8),NZ(8,10)                          LEASTSQ   827
     COMMON/FINL/ TRIX(80,80),RHS(80),R(4,9),ECALC(8,9,9)                LEASTSQ   828
     COMMON /DEVICE/ IIN, IOUT, INCARD, FMT(20),IOUT1,IOUT2,             LEASTSQ   829
    1 IOUT3,IOUT4,MMM,IM,IW,IP,ITT                                       LEASTSQ   830
     DIMENSION BOLD(6),F(8),DB(6),SIGDB(6),DAY(8)                        LEASTSQ   831
44   FORMAT(34H VARIATION OF CAY WITH RESOLUTION ,/,1H ,15X,8F8.5,5X,    LEASTSQ   832
    1 F8.5)                                                              LEASTSQ   833
50   FORMAT(16H A.D.RESIDUALS  8F8.2)                                    LEASTSQ   834
  63 FORMAT(1H1,20A4,//)                                                 LEASTSQ   835
68   FORMAT(31H0RMS ERROR IN F IN GIVEN SIZES )                          LEASTSQ   836
69   FORMAT(1H 10F10.1)                                                  LEASTSQ   837
70   FORMAT(16H RMS DIFFERENCES 8F8.2)                                   LEASTSQ   838
72   FORMAT(1H1)                                                         LEASTSQ   839
  74 FORMAT(1H ,"MINIMUM ZONE SPACINGS FOR SHELLS",/,1H ,15X,8F8.2)      LEASTSQ   840
75   FORMAT(1H 10F10.2)                                                  LEASTSQ   841
76   FORMAT(1H 10F10.0)                                                  LEASTSQ   842
77   FORMAT(30H FIGURE OF MERIT DISTRIBUTION )                           LEASTSQ   843
78   FORMAT(1H )                                                         LEASTSQ   844
  79 FORMAT(10H0COMPOUND I1,5X,2A4)                                      LEASTSQ   845
80   FORMAT (14H NUM PER ZONE 8F8.0)                                     LEASTSQ   846
 81  FORMAT(12H RMS SMALLF 4X,8F8.2)                                     LEASTSQ   847
 82  FORMAT(12H RMS CLOSURE 4X,8F8.2)                                    LEASTSQ   848
  83 FORMAT(16X,8F8.0,5X,F8.0)                                           LEASTSQ   849
```

Plot $\frac{(P(J)}{PMAX}$ vs $J = \Delta\alpha_1$

SUBROUTINE FINAL

TOT = # observations - # variables

CONST = ΣW * EPNSQ = $\Sigma W\epsilon^2$

F(J) = shell = $\frac{1}{GAP}$, $\frac{2}{GAP}$, ...etc.

ie $\frac{\Delta dgap}{n} = F(n)$

Originally

FSIZE(J,2) was input but it was later replaced (LEASTSQ 452) |

FSIZE(J,1) = ΣEPSQ

ESIZE(J,2) = Σ1

```
 84 FORMAT(16H FIG MERIT        ,8F8.4,5X,F8.4)                          LEASTSQ   850
 85 FORMAT(16H R WEIGHTED       ,8F8.4,5X,F8.4)                          LEASTSQ   851
 86 FORMAT(16H R MODULUS        ,8F8.4,5X,F8.4)                          LEASTSQ   852
 87 FORMAT(6F10.6)                                                       LEASTSQ   853
 89  FORMAT(3F10.4,I5,5X,5I1)                                            LEASTSQ   854
 91  FORMAT(8F8.1)                                                       LEASTSQ   855
 92  FORMAT(12H ANOM DISP  4X,8F8.1)                                     LEASTSQ   856
 93  FORMAT(12H DERIV  ES  4X,8F8.1)                                     LEASTSQ   857
 94 FORMAT(2I5,F10.5,2A5)                                                LEASTSQ   858
95   FORMAT(1H F10.4,I10,F10.5,33X,F10.4)                               LEASTSQ   859
 96 FORMAT(8F10.2)                                                       LEASTSQ   860
97   FORMAT(8F8.1)                                                      LEASTSQ   861
 98 FORMAT(I5,2F10.4,I5)                                                 LEASTSQ   862
102 FORMAT(16H NUM PER ZONE     ,8F8.1,5X,F8.1)                          LEASTSQ   863
103 FORMAT(16H AVG LK OF CLOS   ,8F8.2,5X,F8.2)                          LEASTSQ   864
104 FORMAT(16H AVG DERIV FPH    ,8F8.2,5X,F8.2 )                         LEASTSQ   865
105 FORMAT(16H AVG W*(E**2)     ,8F8.2,5X,F8.2)                          LEASTSQ   866
106 FORMAT(16H AVG W*(FPH**2)   ,8F8.2,5X,F8.2)                          LEASTSQ   867
107 FORMAT(16H AVG SMALL F      ,8F8.2,5X,F8.2)                          LEASTSQ   868
108 FORMAT(16H AVG FP(NATIVE)   ,8F8.2,5X,F8.2)                          LEASTSQ   869
109 FORMAT(16H AVG W*(FH**2)    ,8F8.2,5X,F8.2,//)                       LEASTSQ   870
114 FORMAT(16H KRAUT R VALUE  ,8F8.4,5X,F8.4)                            LEASTSQ   871
115 FORMAT(16H L. S. R VALUE  ,8F8.4,5X,F8.4)                            LEASTSQ   872
116 FORMAT(16H CENTRIC R VALUE,8F8.4,5X,F8.4)                            LEASTSQ   873
117 FORMAT(16H AVG DELF N.C.O. ,8F8.2,5X,F8.2)                           LEASTSQ   874
118 FORMAT(16H AVG DELF C.O.   ,8F8.2,5X,F8.2)                           LEASTSQ   875
119 FORMAT(16H NUM CROSS OVERS ,8F8.2,5X,F8.2,//)                        LEASTSQ   876
120 FORMAT(50H STATISTICS FOR GENERAL REFLECTIONS FOR COMPOUND  ,I5,/)   LEASTSQ   877
121 FORMAT(50H STATISTICS FOR CENTRIC REFLECTIONS FOR COMPOUND  ,I5,/)   LEASTSQ   878
122 FORMAT(50H R VALUES FOR GENERAL REFLECTIONS FOR COMPOUND    ,I5,/)   LEASTSQ   879
123 FORMAT(50H R VALUES FOR CENTRIC REFLECTIONS FOR COMPOUND    ,I5,/)   LEASTSQ   880
124 FORMAT(16H RATIO DELF/FPH  ,8F8.2,5X,F8.2)                           LEASTSQ   881
126 FORMAT(16H RMS EST. ERROR ,8F8.2)                                    LEASTSQ   882
140 FORMAT(//)                                                           LEASTSQ   883
150 FORMAT(1H ,11X,"OLD",6X,"DEL",4X,"MAG",8X,"NEW( SIGMA)   INITIAL")   LEASTSQ   884
151 FORMAT(7H ANOM  ,F8.2," + ",F6.2," * ",F4.2," = ",F8.2,"(",F6.2,     LEASTSQ   885
   1")",F10.2,"   CRYST NO",I3)                                          LEASTSQ   886
152 FORMAT(7H   X   ,F8.4," + ",F6.4," * ",F4.2," = ",F8.4,"(",F6.4,     LEASTSQ   887
   1")",F10.4)                                                           LEASTSQ   888
153 FORMAT(7H   Y   ,F8.4," + ",F6.4," * ",F4.2," = ",F8.4,"(",F6.4,     LEASTSQ   889
   1")",F10.4)                                                           LEASTSQ   890
154 FORMAT(7H   Z   ,F8.4," + ",F6.4," * ",F4.2," = ",F8.4,"(",F6.4,     LEASTSQ   891
   1")",F10.4)                                                           LEASTSQ   892
155 FORMAT(7H   R   ,F8.2," + ",F6.2," * ",F4.2," = ",F8.2,"(",F6.2,     LEASTSQ   893
   1")",F10.2)                                                           LEASTSQ   894
156 FORMAT(7H SCALE ,F8.4," + ",F6.4," * ",F4.2," = ",F8.4,"(",F6.4,     LEASTSQ   895
   1")",F10.4,"   CRYST NO",I3)                                          LEASTSQ   896
157 FORMAT(7H BOVER ,F8.2," + ",F6.2," * ",F4.2," = ",F8.2,"(",F6.2,     LEASTSQ   897
   1")",F10.2)                                                           LEASTSQ   898
    TOT=-FLOAT(NVAR)                                                     LEASTSQ   899
    DO 31 M=1,NCPDS                                                      LEASTSQ   900
    DO 31 N=1,8                                                          LEASTSQ   901
31  TOT=TOT+ECALC(M,3,N)                                                 LEASTSQ   902
    CONST=R(3,9)/TOT                                                     LEASTSQ   903
    HIGH=0.0                                                             LEASTSQ   904
    DO 26 J=1,8                                                          LEASTSQ   905
    HIGH=HIGH+GAP                                                        LEASTSQ   906
26     F(J)=1.0/HIGH                                                     LEASTSQ   907
    WRITE(IW,63)TITLE                                                    LEASTSQ   908
    WRITE(IW,68)                                                         LEASTSQ   909
    PRINT 69,  (FSIZE(J,2),J=1,8)                                        LEASTSQ   910
    WRITE(IW,78)                                                         LEASTSQ   911
```

Print FSIZE(J,2) from last cycle where EPSQ

$$= \left\{\left(\frac{SCL}{SHAPE}\right) * F_{PHobs} - F_{PHcalc}\right\}^2 = \varepsilon^2$$

Print out n = # observations in range F_{gap}

Print rms error in each range

$$\text{ie}\sqrt{\frac{\Sigma EPSQ}{n}}$$

$$\varepsilon = \{|F_{PH} - |\bar{F}_p + \bar{f}_j|\}$$

```
      DO 30 J=1,8                                                       LEASTSQ   912
      IF(FSIZE(J,2).EQ.0.0) GO TO 32                                    LEASTSQ   913
      FSIZE(J,3)=FSIZE(J,1)/FSIZE(J,2)                                  LEASTSQ   914
32    FSIZE(J,2)=SQRT(FSIZE(J,3))                                       LEASTSQ   915
30    CONTINUE                                                          LEASTSQ   916
      PRINT 69,  (FSIZE(J,2),J=1,8)                                     LEASTSQ   917
      IF(MARK.EQ.0) PUNCH 97,(FSIZE(J,2),J=1,8)                         LEASTSQ   918
      NV=1                                                              LEASTSQ   919
      LIST=1                                                            LEASTSQ   920
      DO 11 I=1,NCPDS                                                   LEASTSQ   921
      M=NCRYST(I)                                                       LEASTSQ   922
      WRITE(IW,63)TITLE                                                 LEASTSQ   923
      WRITE(IW,79)I,CPDTLE(I,1),CPDTLE(I,2)                             LEASTSQ   924
      WRITE(IW,140)                                                     LEASTSQ   925
      WRITE(IW,74)  ( F(J),J=1,8)                                       LEASTSQ   926
      IF(CAY(I).EQ.0.0) GO TO 40                                        LEASTSQ   927
      S1=0.0                                                            LEASTSQ   928
      S2=0.0                                                            LEASTSQ   929
      DO 42 J=1,8                                                       LEASTSQ   930
      S1=S1+ECALC(I,6,J)                                                LEASTSQ   931
      S2=S2+ECALC(I,7,J)                                                LEASTSQ   932
      DAY(J)=0.0                                                        LEASTSQ   933
      IF(ECALC(I,7,J).EQ.0.0) GO TO 42                                  LEASTSQ   934
      DAY(J)=ECALC(I,6,J)/ECALC(I,7,J)                                  LEASTSQ   935
      ECALC(I,7,J)=ECALC(I,7,J)*CAY(I)*CAY(I)                           LEASTSQ   936
42    CONTINUE                                                          LEASTSQ   937
      CAY(I)=S1/S2                                                      LEASTSQ   938
      WRITE(IW,44)(DAY(J),J=1,8),CAY(I)                                 LEASTSQ   939
   40 CONTINUE                                                          LEASTSQ   940
      IF(MARK.EQ.0) PUNCH 94,NATOM(I),NCRYST(I),CAY(I),CPDTLE(I,1),     LEASTSQ   941
     1 CPDTLE(I,2)                                                      LEASTSQ   942
      DO 12 J=1,8                                                       LEASTSQ   943
      EIS(I,J)=0.0                                                      LEASTSQ   944
      EAD(I,J)=0.0                                                      LEASTSQ   945
      IF(ECALC(I,3,J).EQ.0.0) GO TO 12                                  LEASTSQ   946
      EIS(I,J)=SQRT(ECALC(I,1,J)/ECALC(I,3,J))                          LEASTSQ   947
      IF((CAY(I).EQ.0.0).OR.(ECALC(I,8,J).EQ.0.0)) GO TO 12             LEASTSQ   948
      EAD(I,J)=SQRT(ECALC(I,5,J)/ECALC(I,8,J))                          LEASTSQ   949
 12   CONTINUE                                                          LEASTSQ   950
      PRINT 93,  (EIS(I,J),J=1,8)                                       LEASTSQ   951
      PRINT 92,  (EAD(I,J),J=1,8)                                       LEASTSQ   952
      IF(MARK.NE.0) GO TO 14                                            LEASTSQ   953
      PUNCH 91,(EIS(I,J),J=1,8)                                         LEASTSQ   954
      PUNCH 91,(EAD(I,J),J=1,8)                                         LEASTSQ   955
   14 CONTINUE                                                          LEASTSQ   956
      WRITE(IW,140)                                                     LEASTSQ   957
      WRITE(IW,150)                                                     LEASTSQ   958
      DO 411 J=1,M                                                      LEASTSQ   959
      OLDSCL=1.0/Q(I,J)                                                 LEASTSQ   960
      Q(I,J)=Q(I,J) + RHS(NV)                                           LEASTSQ   961
      SCL=1.0/Q(I,J)                                                    LEASTSQ   962
      SIGSCL=SQRT(CONST*ABS(TRIX(NV,NV)))                               LEASTSQ   963
      SHIFT=SCL-OLDSCL                                                  LEASTSQ   964
      SCL = OLDSCL + AMAGS*SHIFT                                        LEASTSQ   965
      Q(I,J)=1.0/SCL                                                    LEASTSQ   966
      OLDB=BOVER(I,J)                                                   LEASTSQ   967
      DBO=0.                                                            LEASTSQ   968
      IF(IFBOVR( I,J).NE.0) DBO=RHS(NV+1)                               LEASTSQ   969
      BOVER(I,J) = BOVER(I,J) + DBO                                     LEASTSQ   970
      SIGBO = 0.                                                        LEASTSQ   971
      IF(IFBOVR(I,J).NE.0) SIGBO=SQRT(CONST*ABS(TRIX(NV+1,NV+1)))       LEASTSQ   972
      WRITE(IW,156)OLDSCL,SHIFT,AMAGS,SCL,SIGSCL,Q1(I,J),NZ(I,J)        LEASTSQ   973
```

OLDSCL = orig SCL

$$Q_{ij}' = \frac{1}{SCL_{orig}} + r_s$$

$$SCL = 1/\phi_{ij}'$$

$$\sigma SCL = \sqrt{CONST * |a_{ss}|}$$

```
      WRITE(IW,157)OLDB,DBO,AMAGBO,BOVER(I,J),SIGBO,BOVR1(I,J)          LEASTSQ   974
      IF(MARK.EQ.0) PUNCH 98,NZ(I,J),SCL,BOVER(I,J),IFBOVR(I,J)         LEASTSQ   975
  411 NV=NV+1+IFBOVR(I,J)                                               LEASTSQ   976
      N=NATOM(I)                                                        LEASTSQ   977
      DO 15 J=1,N                                                       LEASTSQ   978
      WRITE(IW,140)                                                     LEASTSQ   979
      WRITE(IW,150)                                                     LEASTSQ   980
      DO 415 K=1,M                                                      LEASTSQ   981
      DANUM=RHS(NV)*FLOAT(LABEL(LIST,1))                                LEASTSQ   982
      SIGDAN=FLOAT(LABEL(LIST,1))*SQRT(CONST*ABS(TRIX(NV,NV)))          LEASTSQ   983
      ANMOLD=ANUM(LIST,K)                                               LEASTSQ   984
      ANUM(LIST,K) = ANUM(LIST,K) + DANUM*AMAGA                         LEASTSQ   985
      WRITE(IW,151)ANMOLD,DANUM,AMAGA,ANUM(LIST,K),SIGDAN,ANUM1(LIST,K), LEASTSQ   986
     1 NZ(I,K)                                                          LEASTSQ   987
  415 NV=NV+LABEL(LIST,1)                                               LEASTSQ   988
      DX=RHS(NV)*FLOAT(LABEL(LIST,2))                                   LEASTSQ   989
      SIGDX =FLOAT(LABEL(LIST,2))*SQRT(CONST*ABS(TRIX(NV,NV)))          LEASTSQ   990
      NV=NV+LABEL(LIST,2)                                               LEASTSQ   991
      DY=RHS(NV)*FLOAT(LABEL(LIST,3))                                   LEASTSQ   992
      SIGDY =FLOAT(LABEL(LIST,3))*SQRT(CONST*ABS(TRIX(NV,NV)))          LEASTSQ   993
      NV=NV+LABEL(LIST,3)                                               LEASTSQ   994
      DZ=RHS(NV)*FLOAT(LABEL(LIST,4))                                   LEASTSQ   995
      SIGDZ =FLOAT(LABEL(LIST,4))*SQRT(CONST*ABS(TRIX(NV,NV)))          LEASTSQ   996
      NV=NV+LABEL(LIST,4)                                               LEASTSQ   997
      XOLD=X(LIST)                                                      LEASTSQ   998
      X(LIST)=X(LIST)+DX * AMAGX                                        LEASTSQ   999
      WRITE(IW,152)XOLD,DX,AMAGX,X(LIST),SIGDX,X1(LIST)                 LEASTSQ  1000
      YOLD=Y(LIST)                                                      LEASTSQ  1001
      Y(LIST)=Y(LIST)+DY * AMAGY                                        LEASTSQ  1002
      WRITE(IW,153)YOLD,DY,AMAGY,Y(LIST),SIGDY,Y1(LIST)                 LEASTSQ  1003
      ZOLD=Z(LIST)                                                      LEASTSQ  1004
      Z(LIST)=Z(LIST)+DZ * AMAGZ                                        LEASTSQ  1005
      WRITE(IW,154)ZOLD,DZ,AMAGZ,Z(LIST),SIGDZ,Z1(LIST)                 LEASTSQ  1006
      IF(MARK.EQ.0) PUNCH 96,(ANUM(LIST,K),K=1,M)                       LEASTSQ  1007
      IF(MARK.EQ.0)  PUNCH 89            ,X(LIST),Y(LIST),Z(LIST),      LEASTSQ  1008
     1NTROP(LIST),(LABEL(LIST,LL),LL=1,5)                               LEASTSQ  1009
      NB=NTROP(LIST)                                                    LEASTSQ  1010
      DO 16 K=1,NB                                                      LEASTSQ  1011
      DB(K)=RHS(NV)*FLOAT(LABEL(LIST,5))                                LEASTSQ  1012
      SIGDB(K)=FLOAT(LABEL(LIST,5))*SQRT(CONST*ABS(TRIX(NV,NV)))        LEASTSQ  1013
      NV=NV+LABEL(LIST,5)                                               LEASTSQ  1014
      BOLD(K) = B(LIST,K)                                               LEASTSQ  1015
      B(LIST,K)=B(LIST,K)+DB(K)   * AMAGB                               LEASTSQ  1016
      WRITE(IW,155)BOLD(K),DB(K),AMAGB,B(LIST,K),SIGDB(K),B1(LIST,K)    LEASTSQ  1017
   16 CONTINUE                                                          LEASTSQ  1018
   28 IF(MARK.EQ.0)    PUNCH 87,(B(LIST,K),K=1,NB)                      LEASTSQ  1019
   15 LIST=LIST+1                                                       LEASTSQ  1020
   11 CONTINUE                                                          LEASTSQ  1021
      DO 20 J=1,9                                                       LEASTSQ  1022
      IF(R(2,J).EQ.0.0) GO TO 21                                        LEASTSQ  1023
      R(1,J)=R(1,J)/R(2,J)                                              LEASTSQ  1024
   21 IF(R(4,J).EQ.0.0) GO TO 22                                        LEASTSQ  1025
      R(3,J)=R(3,J)/R(4,J)                                              LEASTSQ  1026
   22 DO 23 M=1,NCPDS                                                   LEASTSQ  1027
      IF(RVAL(M,1,J).EQ.0.0)GO TO 100                                   LEASTSQ  1028
      RVAL(M,2,J)=RVAL(M,2,J)/RVAL(M,1,J)                               LEASTSQ  1029
      RVAL(M,3,J)=RVAL(M,3,J)/RVAL(M,1,J)                               LEASTSQ  1030
      RVAL(M,4,J)=RVAL(M,4,J)/RVAL(M,1,J)                               LEASTSQ  1031
      RVAL(M,5,J)=RVAL(M,5,J)/RVAL(M,1,J)                               LEASTSQ  1032
      RVAL(M,6,J)=RVAL(M,6,J)/RVAL(M,1,J)                               LEASTSQ  1033
      RVAL(M,7,J)=RVAL(M,7,J)/RVAL(M,1,J)                               LEASTSQ  1034
      RVAL(M,8,J)=RVAL(M,8,J)/RVAL(M,1,J)                               LEASTSQ  1035
```

See end of listing for these
Generally simply averaging

```
100 IF(RCEN(M,1,J).EQ.0.0)GO TO 101                                  LEASTSQ  1036
    RCEN(M,2,J)=RCEN(M,2,J)/RCEN(M,1,J)                              LEASTSQ  1037
    RCEN(M,3,J)=RCEN(M,3,J)/RCEN(M,1,J)                              LEASTSQ  1038
    RCEN(M,4,J)=RCEN(M,4,J)/RCEN(M,1,J)                              LEASTSQ  1039
    RCEN(M,5,J)=RCEN(M,5,J)/RCEN(M,1,J)                              LEASTSQ  1040
    RCEN(M,6,J)=RCEN(M,6,J)/RCEN(M,1,J)                              LEASTSQ  1041
    RCEN(M,7,J)=RCEN(M,7,J)/RCEN(M,1,J)                              LEASTSQ  1042
101 IF(ECALC(M,3,J).EQ.0.0) GO TO 23                                 LEASTSQ  1043
    ECALC(M,1,J)=SQRT(ECALC(M,1,J)/ECALC(M,3,J))                     LEASTSQ  1044
    ECALC(M,2,J)=SQRT(ECALC(M,2,J)/ECALC(M,3,J))                     LEASTSQ  1045
    ECALC(M,4,J)=SQRT(ECALC(M,4,J)/ECALC(M,3,J))                     LEASTSQ  1046
    ECALC(M,9,J)=SQRT(ECALC(M,9,J)/ECALC(M,3,J))                     LEASTSQ  1047
    IF((CAY(M).EQ.0.0).OR.(ECALC(M,7,J).EQ.0.0)) GO TO 23            LEASTSQ  1048
    ECALC(M,5,J)=(SQRT(ECALC(M,5,J)/ECALC(M,7,J)))                   LEASTSQ  1049
23  CONTINUE                                                         LEASTSQ  1050
    IF(FIG(2,J).EQ.0.0) GO TO 20                                     LEASTSQ  1051
    FIG(1,J)=FIG(1,J)/FIG(2,J)                                       LEASTSQ  1052
20  CONTINUE                                                         LEASTSQ  1053
    WRITE(IW,140)                                                    LEASTSQ  1054
    PRINT 74,  (F(J),J=1,8)                                          LEASTSQ  1055   minimum zone spacings for shells
    PRINT 86,  (R(1,J),J=1,9)                                        LEASTSQ  1056   R modulus
    PRINT 85,  (R(3,J),J=1,9)                                        LEASTSQ  1057   R weighted
    PRINT 84,  (FIG(1,J),J=1,9)                                      LEASTSQ  1058   mean figure of merit} in shells of 1/GAP
    PRINT 83,  (FIG(2,J),J=1,9)                                      LEASTSQ  1059   number
    WRITE(IW,78)                                                     LEASTSQ  1060   compound
    WRITE(IW,77)                                                     LEASTSQ  1061   figure of merit distribution
    PRINT 76,  (DSTRB(J),J=1,10)                                     LEASTSQ  1062
    DO 25 J=1,10                                                     LEASTSQ  1063
25  DSTRB(J)=0.1*FLOAT(J)-0.05                                       LEASTSQ  1064
    PRINT 75,  (DSTRB(J),J=1,10)                                     LEASTSQ  1065
    DO 24 M=1,NCPDS                                                  LEASTSQ  1066
    WRITE(IW,63)TITLE                                                LEASTSQ  1067
    WRITE(IW,79)M,CPDTLE(M,1),CPDTLE(M,2)                            LEASTSQ  1068
    WRITE(IW,78)                                                     LEASTSQ  1069   compound
    PRINT 74,  (F(J),J=1,8)                                          LEASTSQ  1070   minimum zone spacings for shells
    PRINT 82,  (ECALC(M,1,J),J=1,8)                                  LEASTSQ  1071   rms closure
    PRINT 126,  (ECALC(M,9,J),J=1,8)                                 LEASTSQ  1072   rms estimated error
    PRINT 81,  (ECALC(M,2,J),J=1,8)                                  LEASTSQ  1073   rms small f
    PRINT 80,  (ECALC(M,3,J),J=1,8)                                  LEASTSQ  1074   number per zone
    PRINT 70,  (ECALC(M,4,J),J=1,8)                                  LEASTSQ  1075   rms differences
    WRITE(IW,50)(ECALC(M,5,J),J=1,8)                                 LEASTSQ  1076   a.d. residuals
    WRITE(IW,140)                                                    LEASTSQ  1077
    WRITE(IW,120)M                                                   LEASTSQ  1078   statistics for general reflections for cpd
    PRINT 102,  (RVAL(M,1,J),J=1,9)                                  LEASTSQ  1079   number per zone
    PRINT 103,  (RVAL(M,2,J),J=1,9)                                  LEASTSQ  1080   average lack of closure
    PRINT 104,  (RVAL(M,3,J),J=1,9)                                  LEASTSQ  1081   average deriv FPH
    PRINT 105,  (RVAL(M,4,J),J=1,9)                                  LEASTSQ  1082   average W* (E**2)
    PRINT 106,  (RVAL(M,5,J),J=1,9)                                  LEASTSQ  1083   average W* (FPH**2)
    PRINT 107,  (RVAL(M,6,J),J=1,9)                                  LEASTSQ  1084   average small f
    PRINT 108,  (RVAL(M,7,J),J=1,9)                                  LEASTSQ  1085   average FP (native)
    PRINT 109,  (RVAL(M,8,J),J=1,9)                                  LEASTSQ  1086   average W*(FH**2)
    WRITE(IW,121)M                                                   LEASTSQ  1087   statistics for centric reflections for cpd
    PRINT 102,  (RCEN(M,1,J),J=1,9)                                  LEASTSQ  1088   number per zone
    PRINT 103,  (RCEN(M,2,J),J=1,9)                                  LEASTSQ  1089   average lack of closure
    PRINT 104,  (RCEN(M,3,J),J=1,9)                                  LEASTSQ  1090   average deriv FPH
    PRINT 107,  (RCEN(M,6,J),J=1,9)                                  LEASTSQ  1091   average small f
    PRINT 108,  (RCEN(M,7,J),J=1,9)                                  LEASTSQ  1092   average FP (native)
    PRINT 117,  (RCEN(M,4,J),J=1,9)                                  LEASTSQ  1093   average DELF N.C.O.   no cross overs
    PRINT 118,  (RCEN(M,5,J),J=1,9)                                  LEASTSQ  1094   average DELF C.O.     cross overs
    PRINT 119,  (RCEN(M,8,J),J=1,9)                                  LEASTSQ  1095   number of cross overs
    DO 110 J=1,9                                                     LEASTSQ  1096
    IF(RVAL(M,6,J).EQ.0.0) GO TO 111                                 LEASTSQ  1097
```

```
      RVAL(M,6,J)=RVAL(M,2,J)/RVAL(M,6,J)                                LEASTSQ  1098
  111 IF(RVAL(M,8,J).EQ.0.0) GO TO 112                                   LEASTSQ  1099
      RVAL(M,8,J)=RVAL(M,4,J)/RVAL(M,8,J)                                LEASTSQ  1100
  112 IF(RVAL(M,3,J).EQ.0.0) GO TO 125                                   LEASTSQ  1101
      RVAL(M,2,J)=RVAL(M,2,J)/RVAL(M,3,J)                                LEASTSQ  1102
  125 IF(RVAL(M,5,J).EQ.0.0) GO TO 110                                   LEASTSQ  1103
      RVAL(M,4,J)=SQRT(RVAL(M,4,J)/RVAL(M,5,J))                          LEASTSQ  1104
  110 CONTINUE                                                           LEASTSQ  1105
      WRITE(IW,122)M                                                     LEASTSQ  1106
      PRINT 114,   (RVAL(M,2,J),J=1,9)                                   LEASTSQ  1107
      PRINT 115,   (RVAL(M,4,J),J=1,9)                                   LEASTSQ  1108
      WRITE(IW,86)(RVAL(M,6,J),J=1,9)                                    LEASTSQ  1109
      WRITE(IW,85)(RVAL(M,8,J),J=1,9)                                    LEASTSQ  1110
      DO 130 J=1,9                                                       LEASTSQ  1111
      IF(RCEN(M,6,J).EQ.0.0) GO TO 131                                   LEASTSQ  1112
      RCEN(M,6,J)=RCEN(M,2,J)/RCEN(M,6,J)                                LEASTSQ  1113
  131 IF(RCEN(M,5,J).EQ.0.0) GO TO 132                                   LEASTSQ  1114
      RCEN(M,4,J)=RCEN(M,2,J)/RCEN(M,5,J)                                LEASTSQ  1115
  132 IF(RCEN(M,3,J).EQ.0.0) GO TO 133                                   LEASTSQ  1116
      RCEN(M,2,J)=RCEN(M,2,J)/RCEN(M,3,J)                                LEASTSQ  1117
  133 IF(RCEN(M,3,J).EQ.0.0) GO TO 130                                   LEASTSQ  1118
      RCEN(M,3,J)=RCEN(M,5,J)/RCEN(M,3,J)                                LEASTSQ  1119
  130 CONTINUE                                                           LEASTSQ  1120
      WRITE(IW,140)                                                      LEASTSQ  1121
      WRITE(IW,123)M                                                     LEASTSQ  1122
      PRINT 114,   (RCEN(M,2,J),J=1,9)                                   LEASTSQ  1123
      PRINT 124,   (RCEN(M,3,J),J=1,9)                                   LEASTSQ  1124
      PRINT 116,   (RCEN(M,4,J),J=1,9)                                   LEASTSQ  1125
      WRITE(IW,86)(RCEN(M,6,J),J=1,9)                                    LEASTSQ  1126
   24 CONTINUE                                                           LEASTSQ  1127
      WRITE(IW,72)                                                       LEASTSQ  1128
      RETURN                                                             LEASTSQ  1129
      END                                                                LEASTSQ  1130
      SUBROUTINE MATINV(A,N,B,M,DETERM)                                  LEASTSQ  1131
C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS    LEASTSQ  1132
      DIMENSION IPIVOT(80),A(80,80),B(80,1),INDEX(80,2),PIVOT(80)        LEASTSQ  1133
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)            LEASTSQ  1134
C                                                                        LEASTSQ  1135
C     INITIALIZATION                                                     LEASTSQ  1136
C                                                                        LEASTSQ  1137
   10 DETERM=1.0                                                         LEASTSQ  1138
   15 DO 20 J=1,N                                                        LEASTSQ  1139
   20 IPIVOT(J)=0                                                        LEASTSQ  1140
   30 DO 550 I=1,N                                                       LEASTSQ  1141
C                                                                        LEASTSQ  1142
C     SEARCH FOR PIVOT ELEMENT                                           LEASTSQ  1143
C                                                                        LEASTSQ  1144
   40 AMAX=0.0                                                           LEASTSQ  1145
   45 DO 105 J=1,N                                                       LEASTSQ  1146
   50 IF(IPIVOT(J)-1)60,105,60                                           LEASTSQ  1147
   60 DO 100 K=1,N                                                       LEASTSQ  1148
   70 IF(IPIVOT(K)-1)80,100,740                                          LEASTSQ  1149
   80 IF(ABS(AMAX)-ABS(A(J,K)))85,100,100                                LEASTSQ  1150
   85 IROW=J                                                             LEASTSQ  1151
   90 ICOLUM=K                                                           LEASTSQ  1152
   95 AMAX=A(J,K)                                                        LEASTSQ  1153
  100 CONTINUE                                                           LEASTSQ  1154
  105 CONTINUE                                                           LEASTSQ  1155
  110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM) + 1                                  LEASTSQ  1156
C                                                                        LEASTSQ  1157
C     INTERCHANGE ROWS TO PUT PIVOT ELEMENTS ON DIAGONAL                 LEASTSQ  1158
C                                                                        LEASTSQ  1159
```

R values for general reflections for cpd
Kraut R value
L.S. R value
R modulus
R weighted

R values for centric reflections for cpd

Kraut R value
Ratio DELF/FPH
Centric R value
R Modulus

SUBROUTINE MATINV

```
130 IF(IROW-ICOLUM)140,260,140
140 DETERM=-DETERM
150 DO 200 L=1,N
160 SWAP=A(IROW,L)
170 A(IROW,L)=A(ICOLUM,L)
200 A(ICOLUM,L)=SWAP
205 IF(M)260,260,210
210 DO 250 L=1,M
220 SWAP=B(IROW,L)
230 B(IROW,L)=B(ICOLUM,L)
250 B(ICOLUM,L)=SWAP
260 INDEX(I,1)=IROW
270 INDEX(I,2)=ICOLUM
310 PIVOT(I)=A(ICOLUM,ICOLUM)
320 DETERM=DETERM*PIVOT(I)
C
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
330 A(ICOLUM,ICOLUM)=1.0
340 DO 350 L=1,N
350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT(I)
355 IF(M) 380,380,360
360 DO 370 L=1,M
370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT(I)
C
C     REDUCE NON-PIVOT ROWS
C
380 DO 550 L1=1,N
390 IF(L1-ICOLUM)400,550,400
400 T=A(L1,ICOLUM)
420 A(L1,ICOLUM)=0.0
430 DO 450 L=1,N
450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
455 IF(M) 550,550,460
460 DO 500 L=1,M
500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
550 CONTINUE
C
C     INTERCHANGE COLUMNS
C
600 DO 710 I=1,N
610 L=N+1-I
620 IF(INDEX(L,1)-INDEX(L,2))630,710,630
630 JROW=INDEX(L,1)
640 JCOLUM=INDEX(L,2)
650 DO 705 K=1,N
660 SWAP=A(K,JROW)
670 A(K,JROW)=A(K,JCOLUM)
700 A(K,JCOLUM)=SWAP
705 CONTINUE
710 CONTINUE
740 RETURN
    END
```

```
LEASTSQ  1160
LEASTSQ  1161
LEASTSQ  1162
LEASTSQ  1163
LEASTSQ  1164
LEASTSQ  1165
LEASTSQ  1166
LEASTSQ  1167
LEASTSQ  1168
LEASTSQ  1169
LEASTSQ  1170
LEASTSQ  1171
LEASTSQ  1172
LEASTSQ  1173
LEASTSQ  1174
LEASTSQ  1175
LEASTSQ  1176
LEASTSQ  1177
LEASTSQ  1178
LEASTSQ  1179
LEASTSQ  1180
LEASTSQ  1181
LEASTSQ  1182
LEASTSQ  1183        ECALC(m,1,n) = ΣEPSQ
LEASTSQ  1184
LEASTSQ  1185        ECALC(m,2,n) = ΣFFSQ
LEASTSQ  1186        ECALC(m,3,n) = Σ1.0
LEASTSQ  1187
LEASTSQ  1188        ECALC(m,4,n) = Σ(((F(MCPD)/QT-FP)**2)
LEASTSQ  1189        ECALC(m,5,n) = Σ(ADDIF)^2*WT
LEASTSQ  1190
LEASTSQ  1191        ECALC(m,6,n) = ΣADOBS*ADCALC*WT
LEASTSQ  1192        ECALC(m,7,n) = Σ(ADCALC)^2*WT
LEASTSQ  1193
LEASTSQ  1194        ECALC(m,8,n) = ΣWT
LEASTSQ  1195        ECALC(m,9,n) = Σ((ERNAT*SCALE)**2+(ERR(MCPD)/QT)**2)
LEASTSQ  1196
LEASTSQ  1197
LEASTSQ  1198
LEASTSQ  1199
LEASTSQ  1200
LEASTSQ  1201
LEASTSQ  1202
LEASTSQ  1203
LEASTSQ  1204
LEASTSQ  1205
LEASTSQ  1206
LEASTSQ  1207
LEASTSQ  1208
LEASTSQ  1209
LEASTSQ  1210
LEASTSQ  1211
LEASTSQ  1212
```

Sums from main program (modified in FINAL subroutine). Summations over all reflections.

NORDER = n	RVAL(m,1,n) = Σ1.0	RCEN(m,1,n) = Σ1.0
R(1,n) = ΣABS(EPS)	RVAL(m,2,n) = ΣABS(EPS)	RCEN(m,2,n) = ΣABS(EPS)
R(2,n) = ΣFF	RVAL(m,3,n) = ΣABS(F(MCPD)/QT)	RCEN(m,3,n) = ΣABS(F(MCPD)/QT)
R(3,n) = ΣW*EPNSQ	RVAL(m,4,n) = ΣW*EPNSQ*1.0E6	RCEN(m,4,n) = ΣABS(ABS(FP)-ABS(F(MCPD)/QT))
R(4,n) = ΣW*(FFSQ*(QT**2)	RVAL(m,5,n) = ΣW*(F(MCPD)**2)*1.0E6	RCEN(m,5,n) = ΣABS(ABS(FP)-ABS(F(MCPD)/QT))
	RVAL(m,6,n) = ΣABS(FF)	RCEN(m,6,n) = ΣABS(FF)
	RVAL(m,7,n) = ΣABS(FP)	RCEN(m,7,n) = ΣABS(FP)
	RVAL(m,8,n) = ΣW*(FFSQ*(QT**2)*1.0E6	RCEN(m,8,n) = Σ1.0

FIG(1,n) = ΣFBEST
FIG(2,n) = Σ1.0

$$WT = \left(\frac{QT}{ERR(MCPD)}\right)^2 \qquad QT = \frac{SHAPE}{SCL} \qquad W = \frac{1.0}{QT*QT*EIS(ij)*EIS(ij)+(FSIZE(\ell m))^2}$$

Brookhaven Crystallographic Computer Program

NAME: LIST FILES: 5 TIME: < 77_8 sec

CORE FL: MAX (60K or 30K + 6*NREFLECTIONS)

n ref.	FL
≤ 2000	60K
3000	74K
4000	107K
5000	123K
6000	137K
6800	147K

n.b. the FL is not automatically reduced

Purpose:

LIST is a general program to read the output from a ELINUS FOUR file, sort the reflections according to a user specification, and write the data in a format ready for publication on file ACTA (2000 reflections per journal page). This will appear with 6 columns on the first page of printout followed by 5 on the next. These two segments must be taped together to produce an 11 column matrix which is to be reduced to a 16.5 cm width for ACTA CRYST. Another option is to list the sorted data in a one-dimensional matrix on file SINGLE.

```
PRØGRAM LIST (INPUT,ØUTPUT,FØUR,ACTA,SINGLE,TAPE1=ACTA,
  TAPE2=SINGLE,TAPE20=FØUR)
```

Notes on user options -- The first three integers on the second control card determine how H,K,L will be sorted before the output array is set up. If more than one is non-zero then each of the arrays will be listed on ACTA and SINGLE.

Input:

Card 1 FØRMAT (8A10) (TITLE(8))

Cols. 1-80 title

Card 2 FØRMAT (6I3,F10.0,I10) (IC(I),I=1,6),AMULT,NSID

Cols. 1-3 = 1 The data will be sorted on HKL (H moves slowest)

Cols. 4-6 = 1 The data will be sorted on KHL (K moves slowest)

Cole. 7-9 = 1 The data will be sorted on LHK (L moves slowest)

Cols. 10-12 = 1	This will output an eleven column matrix of data with F(OBS), SIGMA, FCALC in a density of 2000/page.
Cols. 13-15 = 1	Do not include sigma in above output.
Cols. 16-18	Not used.
Cols. 19-28	AMULT = a number by which all values of FO and FC will be multiplied. If left blank it will be assumed to be 10.0.
Cols. 29-38	NSID-- equal to or greater than the number of reflections to be processed (default is 2000, the old maximum).

NOTE - The output on ACTA or SINGLE should be listed on a good line printer with a new ribbon and blank paper. Reasonably good copy can be obtained with reversed paper.

Output:

The output consists of the following:

(1) Title and control information

(2) The number of reflections from FØUR file and output in the various matrices.

(3) The R value for each interval of the slowest moving index and the overall R for all the data.

(4) The data matrices in the configurations desired both on the ØUTPUT file and the special files ACTA and SINGLE.

Note. Each column of output contains 20 characters. The user may find it convenient to vary the distribution of these characters by varying a FØRMAT statement in the subroutine SETUP. For publication efficiency, never use more than a single space between columns.

IMP routine included in library version of program LIST. This routine reads from a standard FLINUS FØUR file.

```
      SUBROUTINE IMP(N,AMULT,J,K,L,FO,FC,SIG,NSID)                      LIST      133
      DIMENSION J(NSID),K(NSID),L(NSID),FO(NSID),FC(NSID),SIG(NSID)     LIST      134
      COMMON/BLATZ/IC(6),TITLE(8),ITAG,HOLM(11,190,2),DUMMY(13)         LIST      135
      COMMON/WOP/NAME(3),MAME(3),BLANK                                  LIST      136
      COMMON/SOP/BUG(3)                                                 LIST      137
C  THIS IS A VARIABLE DATA INPUT SUBROUTINE                             LIST      138
      DO 1 N=2,NSID                                                     LIST      139
       READ(20)J(N),K(N),L(N),SL,FO(N),FC(N),CALPH,SALPH,DELTA,SIG(N)   LIST      140
      IF(EOF(20))4,5                                                    LIST1       5
C  MULTIPLY ALL VALUES OF FOBS AND FCALC BY AMULT                       LIST      142
    5 FO(N)=FO(N)*AMULT                                                 LIST      143
      FC(N)=FC(N)*AMULT                                                 LIST      144
       SIG(N)=SIG(N)*AMULT                                              LIST      145
    1 CONTINUE                                                          LIST      146
    4 N=N-1                                                             LIST      147
      NUMBER=N-1                                                        LIST      148
      PRINT6,NUMBER                                                     LIST      149
    6 FORMAT(* THE NUMBER OF REFLECTIONS CONTAINED IN EACH OF THE FOLLOW LIST      150
     1ING MATRICIES IS*I4/)                                             LIST      151
      REWIND20                                                          LIST      152
      RETURN                                                            LIST      153
      END                                                               LIST      154
```

IMP routine included in library version of program LIST. This routine reads from a standard FLINUS FØUR file.

```
      SUBROUTINE IMP(N,AMULT,J,K,L,FO,FC,SIG,NSID)                      LIST      133
      DIMENSION J(NSID),K(NSID),L(NSID),FO(NSID),FC(NSID),SIG(NSID)     LIST      134
      COMMON/BLATZ/IC(6),TITLE(8),ITAG,HOLM(11,190,2),DUMMY(13)         LIST      135
      COMMON/WOP/NAME(5),MAME(5),BLANK                                  LIST      136
      COMMON/SOP/BUG(3)                                                 LIST      137
C     THIS IS A VARIABLE DATA INPUT SUBROUTINE                          LIST      138
      DO 1 N=2,NSID                                                     LIST      139
       READ(20)J(N),K(N),L(N),SL,FO(N),FC(N),CALPH,SALPH,DELTA,SIG(N)   LIST      140
      IF(EOF(20))4,5                                                    LIST1       5
C     MULTIPLY ALL VALUES OF FOBS AND FCALC BY AMULT                    LIST      142
    5 FO(N)=FO(N)*AMULT                                                 LIST      143
      FC(N)=FC(N)*AMULT                                                 LIST      144
       SIG(N)=SIG(N)*AMULT                                              LIST      145
    1 CONTINUE                                                          LIST      146
    4 N=N-1                                                             LIST      147
      NUMBER=N-1                                                        LIST      148
      PRINT6,NUMBER                                                     LIST      149
    6 FORMAT(* THE NUMBER OF REFLECTIONS CONTAINED IN EACH OF THE FOLLOW LIST      150
     1ING MATRICES IS*I4/)                                              LIST      151
      REWIND20                                                          LIST      152
      RETURN                                                            LIST      153
      END                                                               LIST      154
```

****
****

MULTAN SYSTEM PROVISIONAL WRITE-UP NOVEMBER 1973

****
****

```
***** PREPARATION OF DATA FOR NORMAL ****************************************

  RD 1 FORMAT(20A4) TITLE

CARD 2 FORMAT(5I5,4X,A1,2I5)

 COLS 1-5   NB NUMBER OF POINTS ON WILSON PLOT (.LE.20)
 COLS 6-10  ISCALE =0 TO APPLY OVERALL SCALE FACTOR
                   =1 TO APPLY SEPARATE SCALE FACTOR FOR EACH PARITY GROUP
 COLS 11-15 ILIST  =0 TO SUPPRESS LISTING OF E"S
                   =1 TO OBTAIN   ""     ""
 COLS 16-20 NGP NUMBER OF ATOMIC GROUPS TO BE INPUT (.LE.10)
 COLS 21-25 ICENT  =0 FOR NON-CENTROSYMMETRIC SPACE GROUP
                   =1 FOR CENTROSYMMETRIC      ""   ""
 COL  30    LATT   =P,A,B,C,I,F,R (LATTICE TYPE)
 COLS 31-35 NSYM NUMBER OF SYMMETRY CARDS TO BE INPUT
 COLS 36-40 NREF ""     "" REFLEXIONS TO BE WRITTEN ON MULTAN FILE
 COLS 41-45 DMIN   (DEFAULT VALUE = 1.1)  FOR AUTOMATIC
      46-50 DMAX   (              = 1.9)  INTERPRETATION
      51-55 ANGMIN (              = 85.)  PROGRAM
      56-60 ANGMAX (              =145.)

CARD 3 FORMAT(9F8.0) SCALE FACTOR CARD

       IF PROGRAMME IS TO COMPUTE ITS OWN SCALE AND TEMPERATURE FACTORS,THIS
       CARD SHOULD BE BLANK
 COLS 1-8 TEMP TEMPERATURE FACTOR
          REMAINING 8 FIELDS ARE SCALE FACTORS FOR EEE,OEE,EOE,OOE,EEO,OEO,
        EOO,OOO PARITY GROUPS RESPECTIVELY
          IF ISCALE = 0, FIRST FIELD CONTAINS OVERALL SCALE FACTOR

CARD 4 FORMAT(6F10.6) CELL PARAMETERS

       A,B,C,ALPHA,BETA,GAMMA     (ANGSTROMS AND DEGREES)

CARD 5 FREE FORMAT  NSYM SYMMETRY CARDS

       EACH CARD CONTAINS ONE GENERAL EQUIVALENT POSITION PUNCHED AS
                        1/4-X,Y,1/2+Z
       IF SPACE GROUP IS CENTROSYMMETRIC,DO NOT INCLUDE EQUIVALENT POSITIONS
       RELATED BY THE CENTRE OF SYMMETRY
       IF SPACE GROUP IS CENTRED, INCLUDE ONLY THOSE EQUIVALENT POSITIONS
       ASSOCIATED WITH ONE LATTICE POINT

CARD 6 FORMAT(8(3X,A2,I5)) UNIT CELL CONTENTS

 COLS 4-5  NAT(1,1) CHEMICAL SYMBOL OF ATOMIC TYPE 1 (RIGHT ADJUSTED TO COL.5)
 COLS 6-10 NAT(1,2) NUMBER OF ATOMS OF THIS TYPE IN UNIT CELL
        ETC. TO A MAXIMUM OF 8 ATMMIC TYPES
         THE SCATTERING FACTORS FOR 38 DIFFERENT KINDS OF ATOM ARE STORED IN
         THE PROGRAMME. IN ORDER OF ATOMIC NUMBER THEY ARE
         H,LI,BE,B,C,N,O,F,NA,MG,AL,SI,P,S,CL,K,CA,CR,MN,FE,CO,NI,CU,ZN,AS,SE,
         BR,MO,AG,CD,SN,SB,I,PT,AU,HG,PB,BI
         IF THE ATOMIC SYMBOLS PUNCHED ON THE CARD ARE NOT ONE OF THE ABOVE,
         THE CONSTANTS FOR THE ANALYTICAL SCATTERING FACTOR CURVE CAN BE READ
         FROM THE FOLLOWING CARDS.

CARDS 7 FORMAT(5F10.0) FORSYTH AND WELLS CONSTANTS (ACTA CRYST.(1959).12,412)
```

THESE CARDS ARE INCLUDED ONLY IF AN ATOMIC TYPE DOES NOT CORRESPOND TO ONE OF THE ABOVE AND ARE IN THE ORDER OF APPEARANCE OF THE ATOMS ON CARD 6
THE 5 F. AND W. CONSTANTS ARE PUNCHED IN THE ORDER CAPITAL A,A, CAPITAL B,B,CAPITAL C

RDS 8 FORMAT(1X,A4,I5,F5.0,5X,6F10.3/(3X,A2,3F10.0,45X)) THE NGP ATOMIC GROUPS

IF NGP=0 THESE CARDS ARE NOT INCLUDED
FOR EACH GROUP THE FIRST CARD IS
COLS 2-5 IDENT ALPHANUMERIC CHARACTERS TO IDENTIFY GROUP
COLS 6-10 NT NUMBER OF ATOMS IN GROUP
COLS 11-15 GN NUMBER OF TIMES THIS GROUP IS PRESENT IN THE UNIT CELL
COLS 21-30 A) PARAMETERS OF THE
COLS 31-40 B) CELL TO WHICH
COLS 41-50 C) THE COORDINATES
COLS 51-60 ALPHA) OF THE ATOMS
COLS 61-70 BETA) IN THE GROUP
COLS 71-80 GAMMA) REFER.
THE REMAINING CARDS CONTAIN THE IDENTIFICATION AND COORDINATES OF THE NT ATOMS IN THE GROUP
COLS 4-5 NF CHEMICAL SYMBOL OF ATOM (RIGHT ADJUSTED TO COL.5)
COLS 6-15 X POSITIONAL PARAMETERS OF ATOM
COLS 16-25 Y
COLS 26-35 Z
IF THE FIELDS IN COLS 21-80 OF THE FIRST CARD ARE LEFT BLANK, THE COORDINATES MUST BE GIVEN IN ANGSTROMS FOR AN ORTHOGONAL SYSTEM OF AXES IN WHICH CASE ORIGIN AND ORIENTATION OF GROUP ARE ARBITRARY. OTHERWISE THE FRACTIONAL COORDINATES CORRESPONDING TO THE CELL DEFINED BY A,B,C,ALPHA,BETA,GAMMA ARE GIVEN. THIS ALLOWS THE DIRECT USE OF DATA TAKEN FROM THE LITERATURE.

CARD 9 FORMAT(I5,18A4) FORMAT FOR REFLEXION DATA

COLS 1-5 NNN NUMBER OF REFLEXIONS PUNCHED ON EACH CARD
COLS 6-77 FMT FORMAT FOR READING REFLEXION CARDS

CARD 10 FORMAT AS CARD 9 REFLEXION DATA

FOR EACH REFLEXION, PROGRAMME EXPECTS H K L FOBS ID WHERE ALL ARE INTEGER EXCEPT FOBS
ID=0 FOR OBSERVED REFLEXION
=1 "" UNOBSERVED ""
DATA IS TERMINATED BY DUMMY REFLEXION WITH NEGATIVE FOBS
THE HIGHEST NREF E"S WILL BE WRITTEN ONTO FILE LOUS FOR INPUT TO MULTAN WITH THE RESTRICTION THAT E .GE. 1.0
THE LOWEST 50 E"S WILL ALSO BE WRITTEN ONTO FILE LOUS FOR THE PSI ZERO TEST WITH THE RESTRICTION THAT E .LE. 0.15 AND THETA .LE. 40 DEGREES (CU RADIATION, SIN THETA/LAMDA = .417)

***** PREPARATION OF DATA FOR MULTAN **********

.JR MORE DETAILS SEE MULTAN, A COMPUTER PROGRAMME FOR THE AUTOMATIC SOLUTION OF CRYSTAL STRUCTURES BY MAIN, WOOLSON AND GERMAIN. MAY 1971, UNIV. OF YORK PRINTING UNIT.

CARD 1 FORMAT(20A4) TITLE

CARD 2 FORMAT(I5,5X,6F10.0) IPATH,LATTICE PARAMETERS A,B,C,ALPHA,BETA,GAMMA

IPATH DETERMINES WHICH SECTIONS OF THE PROGRAMME ARE TO BE USED.
= 1 FOR SIGMA2, = 2 FOR CONVERGE, = 4 FOR FASTAN
OR THE SUM OF CODES FOR ANY COMBINATION.
IPATH = 5 IS ILLOGICAL AND NOT ALLOWED BY THE PROGRAMME.
INCLUDE ONLY THOSE DATA CARDS NEEDED FOR THE SECTIONS OF THE PROGRAMME ASKED FOR.
CARDS 3- 7 ARE USED BY SIGMA2.
CARDS 8- 9 ARE USED BY CONVERGE.
CARDS 10-15 ARE USED BY FASTAN.
LATTICE PARAMETERS NEED BE INCLUDED ONLY IF THE NORMAL FILE IS NOT USED FOR DATA INPUT AND IT IS REQUIRED TO GO ON TO COMPUTE AN E-MAP

CARD 3 FORMAT(16I5) UNIT CELL CONTENTS

COLS 1-5 N(1) NUMBER OF ATOMS OF TYPE (1) PER UNIT CELL
COLS 6-10 Z(1) ATOMIC NUMBER OF TYPE (1) ATOMS
.....
COLS 71-75 N(8) NUMBER OF ATOMS OF TYPE (8) PER UNIT CELL
COLS 76-80 Z(8) ATOMIC NUMBER OF TYPE (8) ATOMS
FOR FEWER THAN 8 ATOMIC TYPES, LEAVE THE REST OF THE CARD BLANK
IF THE DATA IS TO BE INPUT FROM NORMAL FILE, THIS CARD SHOULD BE LEFT BLANK. OTHERWISE THE COMPLETE CONTENTS OF THE UNIT CELL ARE PUNCHED.

CARD 4 FORMAT(3I5,4X,A1,I5,5X,F10.0) SIGMA2 PARAMETERS

IF DATA INPUT FROM NORMAL FILE, ONLY ILIST AND NSRMAX NEED BE PUNCHED
COLS 1-5 ILIST =1 TO REQUEST SIGMA2 LISTING
=0 TO SUPPRESS SIGMA2 LISTING
COLS 6-10 NSRMAX MAXIMUM NUMBER OF UNIQUE PHASE RELATIONSHIPS TO BE USED
THE PROGRAMME SETS UP ALL POSSIBLE PHASE RELATIONSHIPS AND SELECTS THE NSRMAX STRONGEST. FROM EXPERIENCE, THE OPTIMUM RATIO OF NUMBER OF PHASE RELATIONSHIPS TO NUMBER OF REFLEXIONS IS ABOUT 7, ALTHOUGH A RATIO AS SMALL AS 4 HAS BEEN USED SUCCESSFULLY ON SEVERAL OCCASIONS. NSRMAX CAN NOT EXCEED KUSER4/3.
COLS 11-15 ICENT =0 FOR NON-CENTROSYMMETRIC SPACE GROUP
=1 FOR CENTROSYMMETRIC SPACE GROUP
COL 20 LATT = P,A,B,C,I,F,R
COLS 21-25 NSYM NUMBER OF SYMMETRY CARDS TO FOLLOW
COLS 31-40 EMIN ALL E VALUES LESS THAN EMIN ARE IGNORED ON INPUT

CARDS 5 FREE FORMAT NSYM GENERAL EQUIVALENT POSITIONS

IF DATA INPUT FROM NORMAL FILE, THESE CARDS SHOULD NOT BE INCLUDED.
OTHERWISE THEY ARE PUNCHED AS 1/2-X,-Y,1/2+Z

CARDS 6 VARIABLE FORMAT REFLEXION DATA

IF DATA INPUT FROM NORMAL FILE, THESE CARDS SHOULD NOT BE INCLUDED.

THE FIRST CARD CONTAINS THE FORMAT STATEMENT.
EACH SUBSEQUENT CARD CONTAINS H,K,L,E
THE LAST CARD CONTAINS A DUMMY REFLEXION WITH A NEGATIVE E VALUE.
THE REFLEXIONS MAY BE INPUT IN ANY ORDER AS THE PROGRAMME DECIDES INTERNALLY ON THE OPTIMUM ORDER FOR PHASE DETERMINATION. HOWEVER, IT SHOULD BE NOTED THAT THE ORDER OF OUTPUT OF REFLEXIONS IN THE E-MAP DATA IS THE SAME AS THE ORDER OF INPUT HERE. THE NUMBER OF REFLEXIONS INPUT MUST BE LESS THAN KUSER3.

CARDS 7 SAME FORMAT AS CARDS 6 THE PSIZERO REFLEXIONS

IF DATA INPUT FROM NORMAL FILE, THESE CARDS SHOULD NOT BE INCLUDED.
EACH CARD CONTAINS H,K,L,E.
THE LAST CARD CONTAINS A DUMMY REFLEXION WITH A NEGATIVE E VALUE.
THE NUMBER OF PSIZERO REFLEXIONS MUST BE LESS THAN THE NUMBER OF REFLEXIONS IN CARDS 6.
IF PSIZERO REFLEXIONS ARE INCLUDED, UNIT ISCRA IS USED FOR TEMPORARY STORAGE OF ARRAYS DURING SIGMA2.
IF NO PSIZERO REFLEXIONS ARE INCLUDED, THE TERMINATING CARD MUST STILL BE PRESENT BUT UNIT ISCRA WILL NOT BE ACCESSED BY THE PROGRAMME.

CARD 8 FORMAT(5I5,5X,F10.0) CONVERGE PARAMETERS

COLS 1-5	LIST	= 1 TO OBTAIN CONVERGENCE MAPPING
		= 0 TO SUPPRESS CONVERGENCE MAPPING
COLS 6-10	NINPUT	NUMBER OF KNOWN PHASES TO BE INPUT
COLS 11-15	NSPEC	NUMBER OF SPECIAL REFLEXIONS NEEDED IN STARTING SET
COLS 16-20	NGEN	"" GENERAL "" "" ""
COLS 21-25	NANY	NUMBER OF REFLEXIONS OF ANY SORT NEEDED IN STARTING SET.

THE REFLEXIONS WHICH WILL APPEAR IN THE STARTING SET WILL BE THOSE THAT ARE NECESSARY FOR ORIGIN DEFINITION, THE SIGMA1 REFLEXIONS, THE NINPUT KNOWN REFLEXIONS AND NSPEC+NGEN+NANY OTHERS TO WHICH ARBITRARY PHASES VALUES ARE ASSIGNED. SPECIAL REFLEXIONS ARE THOSE WHOSE PHASES ARE RESTRICTED TO TWO VALUES SUCH AS 0 AND PI, WHILE THE PHASE OF A GENERAL REFLEXION MAY TAKE ON ANY VALUE. MULTAN WILL GIVE THESE PHASES THE FOUR VALUES +-PI/4 AND +-3PI/4.

COLS 31-40	PROB	ALL SIGNS DETERMINED BY THE SIGMA1 FORMULA WITH A

PROBABILITY GREATER THAN PROB WILL BE ACCEPTED.

CARDS 9 FORMAT(5I5,F10.0) THE NINPUT KNOWN PHASES

COLS 1-5	KODE	CODE NUMBER OF REFLEXION
COLS 6-10	H)	MILLER INDICES OF REFLEXION IN ""STANDARD""
COLS 11-15	K)	FORM AS IT APPEARS IN THE OUTPUT FROM
COLS 16-20	L)	SIGMA2
COLS 21-25	IFAZ	PHASE ANGLE IN DEGREES (+VE ANGLE IN THE RANGE 1-360)
COLS 26-35	WT	

WT=-2.0	ENANTIOMORPH FIXING REFLEXION (IFAZ IGNORED)
WT=-1.0	STARTING SET REFLEXION (IFAZ IGNORED)
WT=0. TO 1.0	KNOWN PHASE
WT=2.0	ORIGIN FIXING REFLEXION

EITHER KODE OR H,K,L SHOULD BE PUNCHED.
APART FROM THIS OBVIOUS PURPOSE, THIS FACILITY OF INPUTTING KNOWN PHASE CAN BE USED TO PERSUADE THE PROGRAMME TO CHOOSE DIFFERENT ORIGIN DEFINING REFLEXIONS IF ONE IS DISSATISFIED WITH ITS ORIGINAL CHOICE.
ONE, TWO, OR THREE ORIGIN DEFINING REFLEXIONS OF ONE"S OWN CHOICE MAY BE READ IN AND IF NECESSARY THE PROGRAMME WILL CHOOSE THE REMAINING REFLEXIONS NEEDED TO COMPLETELY DEFINE THE ORIGIN.

CARD 10 FORMAT(5I5) FASTAN PARAMETERS

COLS 1-5	IMK	NUMBER OF STARTING PHASES TO BE INPUT FROM CARDS
		= 0 IF STARTING PHASES TO BE GENERATED BY PROGRAMME.

```
COLS  6-10  IPRINT = 1 TO OBTAIN LISTING OF FINAL PHASE VALUES.
                   = 0 TO SUPPRESS LISTING OF FINAL PHASE VALUES.
COLS 11-15  IPUB   = 1 IF PHASES ARE SUPPLIED FOR COMPARISON WITH THE PHASES
                       PRODUCED BY THE TANGENT FORMULA. THE PHASES SUPPLIED
                       COULD BE CALCULATED (FOR EXAMPLE) FROM A PUBLISHED
                       STRUCTURE AND THIS FACILITY HAS BEEN FOUND USEFUL IN
                       THE DEVELOPMENT AND TESTING OF MULTAN.
                      SUITABLE FOR COMPUTATION OF E-MAPS (SEE SUBROUTINE FOUR)
                   = 0 IF NO PUBLISHED PHASES ARE SUPPLIED.
COLS 16-20  IFOUR  = 1 TO REQUEST OUTPUT OF PHASES ON UNIT LOUT IN A FORM
                   = 0 IF NO E-MAP OUTPUT REQUIRED, IN WHICH CASE NO TAPE IS
                       NECESSARY ON UNIT LOUT.
COLS 21-25  ISKIP
                   = 0 NORMALLY
                   WHEN RE-SUBMITING A JOB THAT RAN OUT OF TIME, ISKIP SHOULD
                   BE SET TO THE VALUE OF THE IDENTIFICATION NUMBER TAKEN BY
                   THE LAST SET GENERATED - 4 (-4 FOR BUFFER CONSIDERATIONS)

CARDS 11 FORMAT(20F4.0)  THE PUBLISHED PHASES IN DEGREES (IF IPUB = 1) IN ORDER
      OF INPUT OF REFLEXIONS IN CARDS 6.

CARDS 12 FORMAT(20I4)    CODE NUMBERS OF THE IMK STARTING REFLEXIONS

CARDS 13 FORMAT(20I4)    MARKERS     ""     ""     ""     ""     ""

CARDS 14 FORMAT(20F4.0)  WEIGHTS     ""     ""     ""     ""     ""

CARDS 15 FORMAT(20I4)    PHASES (IN DEGREES)       ""     ""     ""     ,NUMSET

      NUMSET = IDENTIFICATION NUMBER OF SET OF PHASES.
      AS MANY CARDS 15 AS DESIRED MAY BE INPUT TO PRODUCE DIFFERENT STARTING
      POINTS FOR THE TANGENT FORMULA, TERMINATED BY NUMSET = 0.
      IF IMK ON CARD 10 IS ZERO, CARDS 12-15 ARE NOT REQUIRED.
      THE MARKERS IN CARDS 13 ARE AS FOLLOWS
           1 FOR GENERAL PHASE
           4 FOR PHASE RESTRICTED TO 45 OR 225 DEGREES
           7 FOR IMAGINARY PHASE ( VALUES OF +- PI/2 ONLY)
          10 FOR PHASE RESTRICTED TO 135 OR 315 DEGREES
          13 FOR REAL PHASE (VALUES 0 OR PI ONLY)
             ETC.
          IF THE MARKER IS NEGATIVE, THE PHASE WILL BE KEPT FIXED DURING PHASE
          DETERMINATION AND ONLY ALLOWED TO VARY DURING THE LAST FEW CYCLES OF
          TANGENT FORMULA REFINEMENT.
```

***** PREPARATION OF DATA FOR PROCEDURE FOURIER *****

..L THE PARAMETERS ARE SET BY PREVIOUS STEPS OR HAVE DEFAULT VALUES SO THAT USUALLY NO DATA CARD IS NECESSARY. THERE IS AN AUTOMATIC SEARCH FOR THE MOST PROBABLE SET OF PHASES.
JUST ONE CONTROL CARD IS NECESSARY (SEE RUNNING THE TEST DATA). IT GIVES THE NAMES OF THE THREE FILES GENERATED BY NORMAL AND MULTAN. AS MANY SUCH CARDS AS ONE DESIRES CAN BE INSERTED IN THE SAME JOB.
HOWEVER ANY OF THE DEFAULT VALUES CAN BE OVERRIDDEN BY THE FOLLOWING CARD WITH FORMAT(4I5,4F5.0)

COLS	DEFAULT VALUES
1-5 NOSET	AUTOMATIC SEARCH FOR THE MOST PROBABLE SET OF PHASES NOT YET DEALT WITH (AS SOON AS IT HAS BEEN DETECTED (WELL BEFORE THE SUCCESSFUL OR UNSUCCESSFUL COMPLETION OF THE PROCEDURE) IT BECOMES AUTOMATICALLY ONE OF THE LESS PROBABLE)
6-10 SCANLEVEL	100
11-15 NPIC	NUMBER OF ATOMS IN ASYMMETRIC UNIT * 1.2
16-20 IPRINT	NO PRINTING OF E-MAP (I.E. DEFAULT IS IPRINT = 0, USE 1 HERE TO GET MAP PRINTED.)
21-25 PRINTING	)
26-30 LIMITS ALONG	) DETERMINED BY PROGRAM
31-35 X, Y, AND Z RESPECTIVELY.	)

OR EXAMPLE, SUPPOSE THAT WHILE RUNNING THE TEST DATA, THE PROGRAMME REACHED .HE FOURIER STAGE BUT THE JOB ABNORMALLY TERMINATED FOR LACK OF TIME. THE MOST PROBABLE SET IS STILL AVAILABLE IF SPECIFIED EXPLICITELY. IN THIS CASE INSERT A CARD CONTAINING A 1 IN COLUMN 5 AS THE DATA CARD FOR PROCEDURE 2.

(SET NUMBER 1 HAPPENS TO BE THE MOST PROBABLE AND CORRECT SET FOR CORTISONE)
ANY OTHER DEFAULT VALUE CAN BE ALTERED IN THE SAME WAY.
THE PRINTING FACILITY (IPRINT=1) IS RARELY USED. THE OUTPUT IS A GRID WITH SECTIONS ALONG Y, X ACROSS THE PAGE AND Z RUNNING VERTICALLY. (ABOUT 3 POINTS PER ANGSTROM). THE NUMERICAL VALUES .GE. SCANLEVEL ARE UNDERLINED WITH **** TO FACILITATE CONTOURING.

***** PREPARATION OF DATA FOR PROCEDURE REFINE (PARTIAL STRUCTURES) **********

CARD 1 FORMAT(20A4) TITLE

CARD 2 FORMAT(I5,2F5.0) NAT,B,PKARL

NAT = NUMBER OF ATOMS IN PARTIAL STRUCTURE
B = TEMPERATURE FACTOR (DEFAULT VALUE = VALUE GIVEN BY NORMAL)
PKARL= FRACTION OF THE TOTAL SCATTERING POWER CONTAINED IN THE FRAGMENT
(SEE KARLE,ACTA CRYST.(1968).B24,182)

CARDS 3 FORMAT(3X,A2,3F10.0)

NAT CARDS EACH CONTAINING CHEMICAL SYMBOL,X,Y AND Z
CHEMICAL SYMBOL MUST BE RIGHT AJUSTED

A MAXIMUM OF 100 PHASES (SATISFYING ABS(FCALC).GE.PKARL*ABS(FOBS) WHERE ABS(FOBS) IS ASSOCIATED WITH AN ABS(E).GE.1.5) ARE REINTRODUCED INTO MULTAN AS A NEW STARTING SET.

FILES

```
                                                  I          I  I
                                                  I          I  I
                                                  I    MUL01 I  I NOR01
                                                  I          I  I
                                                  I          I  I
        ************                              I     ************
        *          * @@SCRA                       I     *          *
        *          *----------                    I     *          *
        *  NORMAL  *         I                    I     *    SF    *
        *          *----------                    I     *          *
        *          *                              I     *          *
        ************                              I     ************
             I                                    I          I
             I                                    I          I
             I NOR01                              I    @@SF  I  I MUL01
             I                                    I          I  I
             I                                    I          I  I
        ************                              I     ************
        *          * @@ISCRA                      I     *          * @@ISCRA
        *          *----------                    I     *          *---------
        *  MULTAN  *         I                    I     *  MULTAN  *         I
        *          *----------                    I     *  PART 3  *---------
        *          *                              I     *          *
        ************                              I     ************
            I  I                                  I          I  I
            I  I                                  I          I  I
      MUL01 I  I FAZ01                            I    MUL01 I  I FAZ01
            I  I                                  I          I  I
            I  I                                  I          I  I
I       ************                              I
I       *          *                              I     TO PROCEDURE FOURIER
I       *          *                              I
I       *  EXPAND  *                              I
I       *          *                              I
I       *          *                              I
I       ************                              I
I            I                                    I
I            I                                    I
I            I @@WW2                              I
I            I                                    I
I            I                                    I
I       ************
I       *          * @@WW3                        P
I       *          *----------                    R
I       *   FFT    *         I                    O
I       *          *----------                    C
I       *          *                              E
I       ************                              D
I            I                                    U
I            I                                    R
             I @@WW4                              E
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P            I
R            I                                   R
O      ************                              E
C      *          *                              F
E      *          *                              I
D      *  SEARCH  *                              N
I      *          *                              E
N      *          *
E      ************                              I
             I                                   I
F            I                                   I
O            I @@WW6                             I
U            I                                   I
R            I                                   I
I      ************                              I
E      *          *                              I
R      *          *                              I
       *  DANFIG  *                              I
I      *          *                              I
I      *          *                              I
I      ************                              I
I            I                                   I
I            I                                   I
I            I @@WW6                             I
I            I                                   I
I            I                                   I
I      ************                              I
I      *          *                              I
I      *          *                              I
I      *   MFRP   *                              I
I      *          *                              I
I      *          *                              I
I      ************                              I
I            I                                   I
I            I                                   I
I            I @@WW6                             I
I            I                                   I
I            I                                   I
I      ************                              I
I      *          *                              I
I      *          *-----MUL01                    I
I      *    SF    *                              I
I      *          *-----NOR01                    I
I      *          *                              I
I      ************                              I
I            I                                   I
I            I                                   I
I            I @@SF                              I
I            I                                   I
I            I                                   I
```

NOR01,MUL01 AND FAZ01 ARE PERMANENT CATALOGUED FILES
ALL THE OTHER ONES ARE SCRATCH FILES

* NOTE ON DANFIG **********

ERS WHO WISH TO OBTAIN ORTHOGONAL COORDINATES FOR BUILDING UP A MODEL ON THE AP DISPLAYED BY DANFIG SHOULD REPLACE STATEMENT 00556200 BY

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605 FORMAT(6X,3H700.63X)                                    00556200
```

* NOTE ON MFRP (MOLECULAR FRAGMENT RECOGNITION PROGRAMME) **********

THIS PART OF THE SYSTEM IS THE NEWEST ONE AND HAS NOT YET BEEN FULLY TESTED.
NO DATA CARDS ARE REQUIRED FOR THIS PROGRAMME.
IT TRIES TO MAKE CHEMICAL SENSE OUT OF THE LIST OF PEAKS OUTPUT BY SEARCH BY USING THE RESTRICTIONS EXISTING ON THE VALUES OF THE INTRAMOLECULAR BOND DISTANCES AND ANGLES.
IN MANY CASES, LOOKING UP THE LIST OF DISTANCES AND ANGLES OUTPUT BY DANFIG HAS BEEN FOUND UNNECESSARY OR GREATLY REDUCED. IN THEORY, MFRP SHOULD BE RUN BEFORE DANFIG BUT EXPERIENCE SHOWS THAT VISUAL INTERPRETATION IS IN SOME CASES STILL PAYING OFF. FOR INSTANCE, DUE TO THE LIMITS FOR ALLOWED VALUES OF BONDS AND ANGLES SET IN THE PROGRAMME (1.1 TO 1.95 ANGSTROMS AND 85 TO 145 DEGREES), IT WILL NOT RECOGNISE LINEAR FRAGMENTS AND 3-MEMBERED RINGS AS WELL AS ATOMS WHICH HAVE A COORDINATION OF 5 OR MORE AND ISOLATED ATOMS AS IN WATER MOLECULES.
THE OUTPUT OF MFRP TELLS WHICH ATOM IS BONDED TO WHICH (ATOM IN COL.1 IS LINKED TO ATOMS IN COLS 2, 3 AND 4) AND LISTS THE FRAGMENTS MAKING CHEMICAL SENSE.
FRAGMENTS WHICH CONTAIN FIVE OR MORE PEAKS ARE INPUT TO SF (ASSUMING ALL ATOMS TO BE CARBON AND B=4)
FOR CORTISONE, PEAKS 13, 30 AND 31 HAVE BEEN ELIMINATED (THEY DO NOT APPEAR IN COL.1) BUT PEAK 27 HAS NOT BECAUSE, ALTHOUGH FALSE, IT MAKES CHEMICAL SENSE WITH ITS NEIGHBOURS.

* NOTE ON SF **********

THE RESIDUAL CALCULATED BY SF IS A PARTIAL RESIDUAL. ONLY THE REFLEXIONS EMBARKED INTO MULTAN ARE TAKEN INTO ACCOUNT.

***** SEPARATING THE PROGRAMMES **********

NORMAL	CARD 00000100	TO CARD	00086468
MULTAN	00086500		00315100
EXPAND	00315200		00354000
FFT	00354100		00508400
SEARCH	00508500		00568300
DANFIG	00568400		00708800
SF	00708900		00738300
FRP	00738400		00793400

* NOTE FOR CDC USERS **********

CDC USERS SHOULD MAKE THE FOLLOWING CHANGES

THE LETTER C SHOULD BE PUNCHED IN COL.1 FOR THE CARDS WHOSE SEQUENCE NUMBER ARE

00318900	00484200	00499100	00508600	00509900	00511900	00539900	00541000
00577900	00589400	00591400	00600700	00610400	00622000	00622300	00630500
641700	00644300	00645600	00678300	00682900	00693800	00696700	00700000
705800	00706400	00786500					

00568500 SHOULD BE IN THE ABOVE LIST

THE LETTER C SHOULD BE REMOVED FROM COL.1 IN THE CARDS WITH SEQUENCE NUMBERS

00319000	00319100	00484300	00484400	00510000	00540000	00541100	00541200
00644400	00706500	00786510	00786520				

```
* NOTE ON CORRECTIONS AND MODIFICATIONS ****************************************

  THE FUTURE, THEY WILL BE COMMUNICATED AS FOLLOWS

      ANY FORTRAN STATEMENT                                              ZZZZZZZZZ
./ DELETE SEQ1=XXXXXXXX,SEQ2=YYYYYYYY

   MEANING
IF CARD ZZZZZZZZ IS ALREADY IN THE DECK,REPLACE IT BY THE NEW ZZZZZZZZ
IF CARD ZZZZZZZZ IS NOT YET IN THE DECK,INSERT IT AT POSITION ZZZZZZZZ
REMOVE CARD XXXXXXXX TO CARD YYYYYYYY FROM THE DECK

THESE CONVENTIONS PERMIT IBM USERS TO CORRECT,RE-COMPILE AND RE-CATALOGUE
DIRECT FROM TAPE IN A SINGLE JOB (EXEC PGM=IEBUPDTE FOLLOWED BY EXEC FORTGCL)



***** ANY DETECTION OF BUG, CONSTRUCTIVE CRITICISM OR COMMENT WILL BE
                                                          GRATEFULLY RECEIVED
```


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NOTES ON THE LOCAL (BNL) VERSION AND PROCEDURES FOLLOW

NOTES ON THE MULTAN SYSTEM AT BROOKHAVEN NATIONAL LABORATORY

THE MULTAN SYSTEM OF PROGRAMS AS ISSUED BY GERMAIN AND UPDATED BY THE CORRECTION SET FROM HIM DATED NOVEMBER/1973 HAS BEEN CHECKED AND FOUND TO WORK SUCCESSFULLY HERE.

THE TEST STRUCTURE (CORTISONE) WAS CORRECTLY SOLVED, BUT NOT IN THE SAME WAY AS INDICATED ON THE SUPPLIED TEST OUTPUT. THE ESSENTIAL DIFFERENCE IS THAT THE CONVERGENCE ROUTINE OF MULTAN MAKES A DIFFERENT DECISION AT ITS FINAL STEP AND HENCE OBTAINS DIFFERENT ORIGIN AND ENANTIOMORPH SPECIFICATIONS. PREDICTABLY THEN,THE STRUCTURE FINALLY FOUND BY SEARCH HAS A DIFFERENT CHIRALITY TO THAT OF GERMAIN AND IS WITH RESPECT TO A DIFFERENT ORIGIN. ALL OTHER ASPECTS OF THE PROGRAM APPEAR TO PRODUCE IDENTICAL RESULTS ON BOTH THE LOCAL CDC 6600 AND GERMAINS IBM/360.

AS WELL AS THE CHANGES IMPLIED BY THE NOTE TO CDC USERS (ABOVE), SEVERAL OTHER SMALL CHANGES WERE APPLIED.

1. PROGRAM CARDS WERE INSERTED, THESE ARE REPRODUCED BELOW FOR REFERENCE.
2. BINARY BLOCKING WAS IMPLEMENTED FOR ALL UNFORMATTED I/O BY INSERTING CALL FTNBIN(1,0,ID) INSTRUCTIONS.
3. THE SIZES OF THE TWO ARRAYS IBUFR AND BUFR IN MULTAN SUBROUTINE CONVEG WERE INCREASED FROM (30,3) AND (30) RESPECTIVELY TO (150,3) AND (150). THIS AVOIDS WRAP-AROUND IN THE SIGMA-TWO LISTING FOR ALL REASONABLE CASES BUT DOES NOT INCREASE THE PROGRAMS CORE REQUIREMENTS.
4. THE DO-LOOP INDEX JJ AT LINE 00311100 IN MULTAN SUBROUTINE CONVEG WAS CHANGED TO JK IN TWO PLACES TO AVOID A CONFLICT WITH THE JJ COUNTER THERE.
5. THE CALL TO ARCOS IN SUBROUTINE ANG OF PROGRAM MFRP HAS BEEN REPLACED BY A CALL TO THE CDC EQUIVALENT ACOS.
6. TO IMPROVE THE USERS CHANCES OF CONCATENATING PROGRAMS CORRECTLY THE LOGICAL UNIT NUMBERS ASSIGNED TO SOME OF THE I/O UNITS HAVE BEEN CHANGED. IN PARTICULAR, UNITS 9 AND 10 IN PROGRAM FFT HAVE INTERCHANGED ROLES, AND PROGRAMS DANFIG AND MFRP NOW ACCESS UNIT 10 RATHER THAN 9 AS BEFORE.
7. PSEUDO DEVICE TLVN HAS BEEN ADDED TO PROGRAM SF AND EQUIVALENCED TO TAPE11,- AGAIN TO FACILITATE CONCATENATION.

MARCH/75

1. THE PROGRAM UPDATES FROM GERMAIN DATED MARCH/74,JULY/74 AND SEP/74 HAVE BEEN APPLIED TO THE SYSTEM.
2. THE CALL FTNBIN(,,) * SEE 2. ABOVE * HAVE BEEN REMOVED.
3. PROGRAM SEARCH HAS BEEN MODIFIED IN TWO RESPECTS--
   A. THE THREE DIMENSIONAL GAUSSIAN INTERPOLATION OF POSITIONS AND HEIGHTS HAS BEEN REPLACED BY A SIMPLE QUADRATIC INTERPOLATION OF POSITIONS ONLY.
   B. THE PEAK SORT ROUTINE WILL NOW CORRECTLY HANDLE UP TO 100 PEAKS.

PROGRAM CARDS FOR THE EIGHT INDEPENDENT PROGRAMS ARE LISTED BELOW.

```
PROGRAM NORMAL(INPUT=200,OUTPUT,TAPE10,TAPE11,TAPE5=INPUT,          00000010
.   TAPE6=OUTPUT)                                                   00000020

PROGRAM MULTAN(INPUT,OUTPUT,TAPE8,TAPE9,TAPE10,TAPE11,              00086498
.   TAPE5=INPUT,TAPE6=OUTPUT)                                       00086499

PROGRAM EXPAND(INPUT=100,OUTPUT,TAPE8,TAPE9,TAPE10,                 00315198
.  TAPE5=INPUT,TAPE6=OUTPUT)                                        00315199

PROGRAM FFT(OUTPUT,TAPE9,TAPE10,TAPE11,TAPE6=OUTPUT)                00354099

PROGRAM SEARCH(INPUT=100,OUTPUT,TAPE9,TAPE10,TAPE5=INPUT,           00508498
.   TAPE6=OUTPUT)                                                   00508499

PROGRAM DANFIG(INPUT=100,OUTPUT,PUNCH=100,TAPE10,                   00568398
.   TAPE5=INPUT,TAPE6=OUTPUT)

PROGRAM MFRP(INPUT=200,OUTPUT=200,TAPE10,TAPE5=INPUT,TAPE6=OUTPUT)  0073839

PROGRAM SF(INPUT=100,OUTPUT,TAPE8,TAPE10,TLVN,                      00708898
.      TAPE5=INPUT,TAPE6=OUTPUT,TAPE11=TLVN)                        00708899
```

PROGRAM	CORE RQD.	TIME (CP)	(PP)
NORMAL	41K (OCTAL)	10 SEC	40 SEC
MULTAN	106K	100	40
EXPAND	67K	3	90
FFT	72K	30	30
SEARCH	121K	30	30
DANFIG	33K	10	30
MFRP	72K	2	25
SF	33K	5	30

NOTE. THESE CORE REQUIREMENTS HAVE BEEN ROUNDED UPWARDS TO THE NEAREST 1K AND THEY ARE FOR THE PROGRAMS ONLY. REMEMBER TO ALLOW 5-6K FOR THE LOADER ON YOUR JOB CARD. THE TIMES LISTED ARE ONLY ESTIMATES AND REFER TO THE CORTISONE TEST DECK SUPPLIED. THIS DECK HAS 1600 REFLECTIONS AND USES 4 SYMMETRY POSITION ON 300 E-S TO PRODUCE 8 STARTING SETS.

STANDARD RUNS AND DATA FLOW.

FOR THE PURPOSE OF ILLUSTRATING THE JOB CONTROL CARDS THE FOLLOWING REE STANDARD PROCEDURES ARE ASSUMED.

1. NORMAL--MULTAN

2. EXPAND--FFT--SEARCH--DANFIG--MFRP

3. SF--MULTAN(STAGE 3)--EXPAND--FFT--SEARCH--DANFIG---MFRP

EXPLANATION OF THE REQUEST,ATTACH,AND CATALOG CONTROL CARDS MAY BE FOUND IN THE APPROPRIATE SCOPE REFERENCE MANUAL.

ACCESS IS A PROGRAM (WRITTEN BY HJ BERNSTEIN) WHICH ATTACHES THE DESIRED FILE FROM A DISK IF AVAILABLE OTHERWISE THE MASTER COPY IS CALLED IN FROM TAPE.

PROCEDURE 1 CONTROL CARDS -- ASSUMING REFLECTION DATA ON CARDS.

```
ACCOUNT(USERNAME,ACCTNO)
ATTACH(ACCESS,ID=CPROGS)
ACCESS(NORMAL,ID=CPROGS)
ACCESS(MULTAN,ID,CPROGS)
RETURN(ACCESS)
REQUEST(TAPE8,*PF) FOR SIGMA-TWO AND CONVERGE RESULTS FROM MULTAN
REQUEST(TAPE9,*PF) FOR PHASED E OUTPUT FROM MULTAN TO EXPAND
 EQUEST(TAPE10,*PF) FOR HIGH E AND PSIZERO OUTPUT FROM NORMAL
 ORMAL.
RETURN(NORMAL)
RETURN(NML)
REWIND(TAPE8,TAPE9,TAPE10,TAPE11)
CATALOG(TAPE10,NORMALEOUTPUT,ID=JOEUSER,RP=10)
MULTAN.
RETURN(MULTAN,TAPE11)
REWIND(TAPE8,TAPE9)
CATALOG(TAPE8,MULTANSIG2CONV,ID=JOEUSER,RP=10)
CATALOG(TAPE9,MULTANPHASES,ID=JOEUSER,RP=10)
7/8/9
DATA FOR NORMAL
7/8/9
DATA FOR MULTAN
7/8/9
6/7/8/9
```

PROCEDURE 2 CONTROL CARDS

```
JOD CARD
ATTACH(ACCESS,ID=CPROGS)
ACCESS(EXPAND,ID=CPROGS)
 :CESS(FFT,ID=CPROGS)
 :CESS(SEARCH,ID=CPROGS)
ACCESS(DANFIG,ID=CPROGS)
ACCESS(MFRP,ID=CPROGS)
RETURN(ACCESS)
ACCOUNT(USERMAME,ACCTNO)
CARD TO LOCALISE TAPE8 FROM BEFORE E.G. ATTACH(TAPE8,MULTANSIG2CONV,ID=JOEUSER)
CARD TO GET TAPE9 FROM BEFORE, WITH LFN OTHER THAN TAPE9 E.G. ASSUME T9 IS USED
AS THE LFN THEN ACCESS WITH  ATTACH(T9,MULTANPHASES,ID=JOEUSER)
REWIND(TAPE8,T9)
COPYCF(T9,TAPE9)
RETURN(T9)
REWIND(TAPE9)
EXPAND.
REWIND(TAPE9,TAPE10)
RETURN(EXPAND,TAPE8)
FFT.
RETURN(FFT)
REWIND(TAPE9,TAPE10)
SEARCH.
RETURN(SEARCH)
RETURN(SCH)
REWIND(TAPE9,TAPE10)
CARD TO LOCALISE OBJECT CODE FOR DANFIG E.G. ATTACH(DNFG,DANFIG,ID=CPROGS)
RETURN(DANFIG)
REWIND(TAPE9,TAPE10)
MFRP.
RETURN(MFRP)
REWIND(TAPE10)  OPTIONAL
COPYBF(TAPE10,PUNCH)  OPTIONAL
7/8/9
DATA CARD TO OVERIDE DEFAULT PARAMETERS IN PROCEDURE FOURIER, IF DESIRED (THIS
 CARD IS READ BY EXPAND) . IF DEFAULT VALUES ARE DESIRED OMIT THIS CARD  DO NOT
 USE A BLANK.
7/8/9
6/7/8/9
```

PROCEDURE 3 CONTROL CARDS

```
 DB CARD
 CCOUNT(USERNAME,ACCTNO)
ATTACH(ACCESS,ID=CPROGS)
ACCESS(SF,ID=CPROGS)
ACCESS(MULTAN,ID=CPROGS)
ACCESS(EXPAND,ID=CPROGS)
ACCESS(FFT,ID=CPROGS)
ACCESS(SEARCH,ID=CPROGS)
ACCESS(DANFIG,ID=CPROGS)
ACCESS(MFRP,ID=CPROGS)
RETURN(ACCESS)
CARD TO LOCALISE TAPE8 SAVED FROM MULTAN WITH LFN OTHER THAN TAPE8 E.G. --
ATTACH(T8,MULTANSIG2CONV,ID=JOEUSER)
COPYBF(T8,TAPE8)
RETURN(T8)
REWIND(TAPE8)
CARD TO LOCALISE TAPE9 FROM MULTAN  WITH DIFFERENT LFN  E.G. --
ATTACH(T9,MULTANPHASES,ID=JOEISER)
COPYBF(T9,TAPE9)
RETURN(T9)
REWIND(TAPE9)
CARD TO REGAIN TAPE10 FROM NORMAL E.G. ATTACH(TAPE10,NORMALEOUTPUT,ID=JOEUSER)
CARD TO GET OBJECT CODE FOR PROGRAM SF E.G. ATTACH(SF,SF,ID=CPROGS)
SF.
RETURN(SF,TAPE10)
REWIND(TAPE8,TAPE9,TLVN)     TLVN IS THE SF OUTPUT FILE
RETURN(MULTAN,TLVN)
REWIND(TAPE8,TAPE9)
EXPAND.
RETURN(EXPAND,TAPE8,TAPE9)
REWIND(TAPE10)
FFT.
RETURN(FFT)
REWIND(TAPE9,TAPE10)
SEARCH.
RETURN(SEARCH)
REWIND(TAPE9,TAPE10)
DANFIG.
RETURN(DANFIG)
REWIND(TAPE9,TAPE10)
MFRP.
RETURN(MFRP,TAPE9)
REWIND(TAPE10)  OPTIONAL
COPYBF(TAPE10,PUNCH)  OPTIONAL
7/8/9
DATA CARDS FOR SF
7/8/9
DATA CARD TO OVERIDE DEFAULT VALUES IN PROCEDURE FOURIER, IF DEFAULTS ARE
WANTED OMIT THIS CARD DO NOT USE A BLANK
7/8/9
/7/8/9
```

BRIEF PROGRAM DESCRIPTION

NORMAL	READS REFLECTION DATA AND PRODUCES E-S AND STATISTICS
MULTAN	MULTIPLE SOLUTION TANGENT FORMULA METHOD -SEE REFERENCES
EXPAND	EXPANDS MULTAN OUTPUT TO A FULL HEMISPHERE
FFT	THE TEN EYCK PROGRAM FOR CRYSTALLOGRAPHIC FAST FOURIER TRANSFORMS SEE REFERENCES
SEARCH	SCANS THE FFT OUTPUT FOR PEAKS, DECIDES ON THE MOST LIKELY DIRECTION OF LEAST OVERLAP FOR VIEWING AND PRODUCES AN ORTEP STYLE INPUT FILE. FOR DANFIG TO READ.
DANFIG	A LINE-PRINTER VERSION OF ORTEP, DOES A DISTANCE AND ANGLE SCAN AND PLOTS THE PEAK POSITIONS ON THE LINE PRINTER .
MFRP	READS THE SEARCH OUTPUT FILE AND APPLIES KNOWN BOND LENGTHS AND ANGLES TO THE PEAKS IN AN ATTEMPT TO RECOGNIZE MOLECULAR FRAGMENTS, MFRP OVERWRITES ITS OWN INPUT FILE (TAPE10).
SF	ACCEPTS A SET OF PEAK POSITIONS FROM THE USER AND CALCULATES STRUCTURE FACTORS FOR THE HIGH E-S, PRODUCES AN INPUT FILE FOR MULTAN(STAGE 3) - HENCE RECYCLING.

REFERENCES

1 GERMAIN AND WOOLFSON,1968,ACTA CRYST.,VOL B24,PAGE 91.
2 GERMAIN,MAIN,AND WOOLFSON,1970,ACTA CRYST.,VOL A27,PAGE368.
3 GERMAIN,MAIN,AND WOOLFSON,1971,ACTA CRYST.,VOL A28,PAGE 368.
4 DEBAERDEMAEKER AND WOOLFSON,1972,ACTA CRYST.,VOL A28,PAGE 477.
5 DECLERQ,GERMAIN,MAIN,AND WOOLFSON,1973,ACTA CRYST., VOL A29,PAGE 231.
6 M.H.J. KOCH, 1974, ACTA CRYST., VOL B30, PAGE 67.
7 L.F. TEN EYCK,1973,ACTA CRYST., VOL B29,PAGE 183.

BNL WRITE-UP OF FEB/74 GJB WILLIAMS. (UPDATED SEPT./74)

NAME: NANØVA AUTHOR: L. Andrews

CORE: 77K DATE: September 1973

```
PRØGRAM NANØVA(INPUT,ØUTPUT,FØUR,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE3,
               TAPE4=FØUR,TAPE10)
```

I. PURPOSE:

To analyze for correlations between DELTA/SIG and FØBS and between DELTA/SIG and $\sin\theta/\lambda$

II. TAPES:

A. FØUR-Binary	Purpose-input	Format-IH,IK,IL,FØ,FC, SI,DEL,SIGMA
B. TAPE10-Calcomp	Purpose-output	

III. LIMITATIONS:

A. Number of $\sin\theta/\lambda$ and FØBS intervals	Dimension-50
B. Reflection data	Dimension-5000

IV. REPLACEABLE SUBROUTINES:

none

V. DECK SET UP

A. JOB CARD

1. TIME LIMIT - <50 cp secs
2. FIELD LENGTH - $77K_8$
3. NUMBER OF TAPES - 0-2
4. ECS - none

B. CONTROL CARDS

```
ATTACH(NANØVA,NANØVA,ID=CPRØGS)
REQUEST(FØUR,,,)              NOTE: This requests input tape.
REQUEST(TAPE10,,,)            NOTE: This requests calcomp tape.
NANØVA.
```

C. DATA CARDS:

CARD	FØRMAT
1. Title card	9A6
2. Control card 1	24I3
3. Terminator	blank

D. REMOTE FILES:

1. ØUTPUT

Brookhaven Crystallographic Computer Program

NAME: NANOVA TIME: <50 SEC
CORE FL: $77K_8$

PRØGRAM NANØVA(INPUT,ØUTPUT,FØUR,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE3,
TAPE4=FØUR,TAPE10)

NANOVA is a special purpose version of HANOVA. It will analyze for any correlations between DELTA/SIG and FOBS and between DELTA/SIG and SINT/L. The program is designed to require as little user specification as possible, and produces a short ØUTPUT file which can be printed conveniently on a teletype. The FØUR file from FLINUS should be input as file FØUR. If plots are desired before and after the least squares then logical TAPE10 must be mounted and submitted to CALCØMP after job has run. N.B. See page 3 for advice on use.

Limitations on this version of HANOVA are

(1) The max number of independent effects is 50 (i.e. the number of intervals of SINT/L + number of intervals of FOBS cannot exceed 50).

(2) The max number of reflections presently allowed for is 5000.

Data Cards

Card 1 Title (9A6)

Col. 1-54 Any Alphameric information

Card 2 IC(I), I=1,24 (2413)

Col. 1-3 IC(1)=2 always

Col. 4-6 IC(2)=0 always

Col. 7-9 IC(3)=0 always

Col. 10-12 IC(4)=0 for no output of intermediate information
=1 for output of intermediate information
for teletype output always set IC(4)=0

Col. 13-15 IC(5)=0 always

Col. 16-18 IC(6)= the number of data to be included in each interval of FOBS (remember that the total number of intervals must be $\leq$ 50).

Col. 19-21 IC(7)=0 to obtain 4 plots (2 of the data and 2 of results) (TAPE10 must be mounted)
=1 to skip plotting sections (TAPE10 may be skipped)

Col. 22-24 IC(8)=0 always

Col. 25-27 IC(9)=0 or 1 for normal operation
=2 to reduce number of SINT/L intervals
=3 for further reduction of the above
(This is a useful option for very small data sets, when some SINT/L intervals could contain no reflections.)

IC(10)-IC(24) are available for use in DATAIN subroutine

Card 3 Terminator

Blank card for termination

Tapes:
FØUR
TAPE10

Output

The output consists of the following:

(1) The data sorted on increasing FOBS. (every 200-th if ICN(4)=0)

(2) The number of levels in class 1 (the number of intervals of SINT/L).

(3) The number of levels in class 2 (the number of intervals of FOBS).

(4) The limiting values of SINT/L and FOBS for each level.

(5) The matrix of normal equations and its inverse, if IC(4)=1.

(6) The solution to the least squares.

(7) The average value of DELTA/SIG for each interval(level) of SINT/L and FOBS.

(8) The F statistics for the two classes.

SAMPLE DECK SETUP

1. Job Card

Time Limit = 50_8 sec
Field Length = $77K_8$ words
Line Limit = $2K_8$ lines
No. of Tapes = 0-2

2. Control Cards

```
ATTACH(NANØVA,NANØVA,ID=CPRØGS)
REQUEST(FØUR,,,)
REQUEST(TAPE10,,,)
(N.B. REQUEST TAPE10 for calcomp plots only if
IC(7)=0; in this case number of tapes = 2)
NANØVA.
```

3. Data Cards

As described above

Method

The observation analyzed in the analysis of variance program is ABS(DELTA/SIG), where DELTA and SIG are read from file FØUR. Thus, if the SIG on the tape is that used in the least squares refinement, a proper weighting scheme will show an absence of significant effects when classified according to scattering angle and intensity. If the weighting scheme does not appear to be adequate (based on large values of F in the hypothesis tests), the best procedure is as follows:

(1) Prepare a new FØUR file, with SIG=1 for all reflections. This will of course cause DELTA/SIG=DELTA.

(2) Rerun NANØVA, thus analyzing DELTA

(3) If there is a significant trend in only one of the variables, the mean values of ABS(DELTA/SIG) may be used directly as the new sigmas for the observations in that class. It often occurs that the only significant variation is with intensity, not with scattering angle, so that this approach is valid.

(4) If there are significant trends with both variables, a composite weighting scheme may be made up from the table of least squares parameter values using the following formula

$$\sigma = \text{MEAN(ABS(DELTA/SIG))} = A + \text{EFFECT(I)} + \text{EFFECT(J)}$$

I = SINT/L LEVEL
J = FOBS LEVEL
A is a quantity output by NANØVA and is related to the overall mean ABS(DELTA/SIG)

The new weighting scheme should also be tested for reasonableness. Also, any trends or odd-ball points should be examined carefully to reveal the effects of systematic error.

Note: The F_{OBS}'s used by NANØVA are from the FØUR tape. Their scale factor is determined by IWSØ in FLINUS. If a scale has been applied to FOBS on the FØUR tape, it is important to remember that the scaled data (F_{obs} and σ) are analyzed by NANØVA. Use care if you return a NANØVA weighting scheme to FLINUS.

NAME: ØMULT AUTHOR(s): G. Germain

CORE: 110K DATE: March, 1974

PROGRAM ØMULT(INPUT,ØUTPUT,ES,FØUR,INRES,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE90=ES,
TAPE42=FØUR,TAPE74=INRES,TAPE58,SHØRT1=200,TAPE18=SHØRT1,SHØRT2=200,TAPE19=SHØRT2)

I. PURPOSE: This is the old MULTAN program which has been superceded by the new package of eight programs. It will remain available for the time being, since it offers the abbreviated files SHØRT1 and SHØRT2 designed to facilitate use from keyboard terminals. Those wishing to use ØMULT should consult the original MULTAN writeup (May 1971) from York and Louvain.

II. TAPES:

A. FØUR-Binary	Purpose-output	Format-one file for each solution-JH,JK, JL,DUMMY,COS ,SIN ,DUMMY ,DUMMY.
B. INRES-Binary	Purpose-intermediate convergence output, Σ2 output, + input	
C. ES-BCD	Purpose-intermediate Σ1 information input	

III. LIMITATIONS:

	DIMENSION
A. total # of reflections	500
B. Atom types	10
C. No. of Σ2 relationships	2000

IV. REPLACEABLE SUBROUTINES:

	ARGUMENT
FØUR	FOM-to change output for FØUR (see listing)

V. DECK SET UP

A. JOB CARD
1. TIME LIMIT -
2. FIELD LENGTH - 110K
3. PRINT LIMIT -
4. NUMBER OF TAPES - 0-3
5. ECS - 0

B. CONTROL CARDS

```
ATTACH(MULTAN,ØMULT,ID=CPRØGS)
REQUEST(FØUR,,,)
REQUEST(INRES,,,)
REQUEST(ES,,,)
MULTAN.
```

C. DATA CARDS:

CARD	FORMAT
see writeup	

D. REMOTE FILES:

A. SHØRT1
B. SHØRT2

PRØGRAM ØRTEP2(INPUT,ØUTPUT,TAPE3,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE11,TAPE15=TAPE11,PUNCH)

SUPPLEMENTARY INSTRUCTIONS FOR THE OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM ORTEP-II

C. K. Johnson

15 March 1971

ORTEP-II differs from the previously distributed version of ORTEP by a new feature which solves the overlap (hidden-line) problem to eliminate most of the manual touch-up tasks. All of the previous instructions for ORTEP, described in the instruction manual ORNL-3794 (1965; second revision, 1970) remain in effect for ORTEP-II.

The overlap feature requires an additional block of approximately 15 K words of computer memory and will cause ORTEP to exceed the memory available in a 32 K computer. For such a computer, the overlap feature may be deleted by removing subroutines LAP500, LAP700, LAP800, LAPDRW, LAPAB and LAPCON and by substituting dummy subroutines for the first four of these six subroutines.

Drawings made with the overlap correction (instruction 511) activated require up to three times the computing time of non-corrected drawings; consequently, the overlap instruction should not be used for preliminary drawings which involve large numbers of atoms.

Three basic steps are involved in the overlap calculation: (A) the projected-outline storage step, (B) the area-overlap search step, and (C) the hidden-line-segment search step.

Efficient utilization of the overlap correction feature requires that these steps be examined in some detail.

A. The Projected-Outline Storage Step

The projected-outline storage step is controlled by instruction 511 and is executed principally by subroutine LAP500. This step must be performed after the orientation and scaling steps (controlled by instruction 501-504 and 601-614) and before the atom and bond plotting steps (controlled by the 700 and 800 series instructions). The storage step must be re-executed after any changes in orientation or scale, including the stereoscopic rotation (controlled by instruction 503), before plotting the next drawing. The following calculations are performed in the storage step.

(1) The ATOMS list is sorted so that atoms farthest from the viewpoint occur first in the list.

(2) The outline ellipse of each atom in the ATOMS list is projected onto the drawing plane and stored in analytical form in array CONIC along with the minima and maxima in x and y of a rectangle enclosing the ellipse. Up to 500 projected atoms can be stored.

(3) Each bond which is to be included in the overlap calculation is approximated by a quadrangle projected onto the drawing plane and stored in array QUAD. The bonds to be stored are defined by type 2 trailer cards included with the 511 overlap instruction. In general, the entire set of all bonds described by the combined type 2 trailer cards from all the 802/812

instructions should be stored; however, any or none of this set may be used instead, particularly if the omitted bonds are made completely black so that they automatically cover other elements by blacking them out. The maximum number of projected bonds which can be stored is 599.

A constant width overlap margin (i.e., blank area at intersections of overlapping elements) is included in each projected atom ellipse and each projected bond quadrangle. The width of this margin may be specified with the 511 instruction if desired; otherwise, the margin is set by default to either 0.025 inch or $\sqrt{\text{SCAL1}}$ x 0.030 inch, whichever is largest. Some users prefer an overlap margin of 0.0 for stereoscopic drawings.

All information stored by the 511 instructions is deleted whenever a 501-510 or 600 series instruction is executed. The 511 instruction card has the following format.

Columns		
3	2	- if bonds are to be stored; otherwise, blank or zero.
7-9	511	
10-18	blank or zero	- overlap margin default option described above.
	1 (or -1)	- overlap margin = 0.0
	0 < OVMRGN < 1.0	- overlap margin (in inches).

The 511 instruction card is followed by type 2 trailer cards unless col. 3 is blank. (In general, all of the type 2 trailer cards included with the 802/812 instruction cards are used.)

The remaining steps, B and C, of the overlap routine are carried out automatically.

B. The Area-Overlap Search Step

This step is executed automatically just before each atom or stick bond is drawn by the 700/800 series of instructions. A search is made of the stored projected atom ellipse and bond quadrangle arrays to compile a list of up to twenty interfering atoms plus thirty interfering bonds which overlap the atom or bond to be drawn. The atom-over-atom search is done by subroutine LAP700, the bond-over-bond search by subroutine LAP800, and the atom-over-bond and bond-over-atom searches by subroutine LAPAB.

C. The Hidden-Line-Segment Search Step

All the graphical constructions used by ORTEP are composed of straight-line segments. An ellipse, for example, is approximated by 16 to 128 straight-line segments depending upon the size of the ellipse. Before each line segment in the graphical representation of an atom or bond is drawn, a search of the stored interfering elements found in the area-overlap search step is made by subroutine LAPDRW and a list is compiled of all intersections of the line segment with the interfering ellipses and quadrangles. The intersection list is sorted according to distance along the line segment and the overlap pattern is analyzed to determine which parts of the line segment are visible. Finally, the visible portions are drawn.

An important feature of the ORTEP-II scheme for correcting overlap is that all details inside atoms and bonds, including

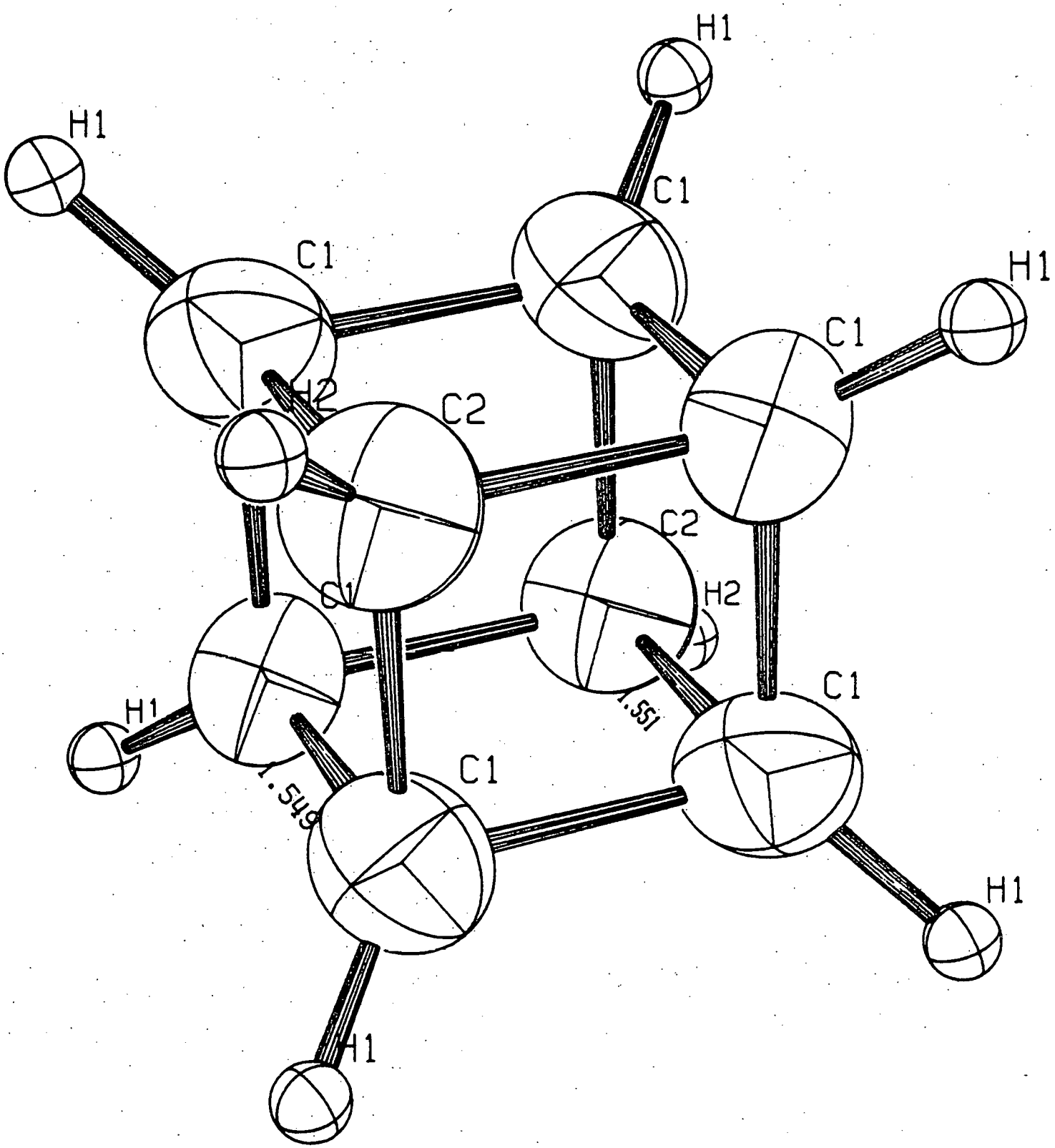
chemical symbols and bond-distance labels, will be corrected for overlap; however, note that chemical symbols (drawn by the 700 instructions) and bond-distance labels (drawn by the 802/812 instructions) which are outside the atom or bond may not be corrected for overlap, since the area-overlap search step does not save interfering elements which are completely outside the atom or bond. Labels and symbols drawn with the 900 series instructions will not be corrected for overlap.

The mathematics of the overlap calculation is not so trivial as it may seem at first glance; however, the problems involved are all classical and the answers are available in concise form in the rich, but currently rather neglected, field of projective geometry. The text by C. E. Springer entitled Geometry and Analysis of Projective Spaces, Freeman and Co., (1964), and the text by J. A. Todd entitled Projective and Analytical Geometry, Pitman Publ. Corp., 1946, are useful references.

A listing of the data and instruction cards for a stereoscopic drawing of Cubane with overlap correction is given below as an example problem for ORTEP-II. The unretouched right-eye member of the Cubane stereo pair is shown.

```
 CUBANE  E.B.FLEISCHER   1964  J.A.C.S.  86,3889                          EXAM0010
     5.34     5.34     5.34    72.26    72.26    72.26                    EXAM0020
              0  1  0  0              0  0  1  0              0  0  0  1EXAM0030
              0  0  0  1              0  1  0  0              0  0  1  0EXAM0040
              0  0  1  0              0  0  0  1              0  1  0  0EXAM0050
              0 -1  0  0              0  0 -1  0              0  0  0 -1EXAM0060
              0  0  0 -1              0 -1  0  0              0  0 -1  0EXAM0070
1             0  0 -1  0              0  0  0 -1              0 -1  0  0EXAM0080
  C1                            -.18711   .19519   .10706        0        EXAM0090
   .04100   .04250   .04500   -.00420  -.01420  -.00510        0        EXAM0100
  C2                             .11546   .11546   .11546        0        EXAM0110
   .04680   .04680   .04680   -.01430  -.01430  -.01430        0        EXAM0120
  H1                            -.32460   .34680   .18480        0        EXAM0130
      .10                                                        7        EXAM0140
  H2                             .21000   .21000   .21000        0        EXAM0150
      .10                                                        7        EXAM0160
 ORGN                                 0        0        0        0        EXAM0170
1                                                               0        EXAM0180
  3   101   155501        2        1        4     3.61                   EXAM0190
***** FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A *****       EXAM0200
  3   102   155501        2        1        4      1.8                   EXAM0210
***** FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS *****           EXAM0220
  3   201                                                               EXAM0230
***** INITIALIZE MECHANICAL PLOTTER PACKAGE. 203 FOR CRT PACKAGE *****   EXAM0240
  3   301      11.      11.      30.      1.5                            EXAM0250
***** 11X11 BOUNDARY, 8X8 INSIDE 1.5 MARGIN, VIEW FROM 30 INCHES *****   EXAM0260
  3   303                                                               EXAM0270
***** ELIMINATE ALL RETRACING *****                                      EXAM0280
  3   402   555501        5        1        4      3.2                   EXAM0290
***** ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01 *****    EXAM0300
  3   501   555501   255501   155501   255501   155502                 0EXAM0310
***** ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE *****EXAM0320
  3   502        2      25.        1      28.                           EXAM0330
***** ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X *****       EXAM0340
  3   604        0        0        0     1.54                           EXAM0350
***** AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS **EXAM0360
```

```
  3   503        2       2.7                                                EXAM0370
***** STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE *****             EXAM0380
  3  1101                                                                   EXAM0390
***** START SAVE SEQUENCE *****                                             EXAM0400
  2   511        0                                                          EXAM0410
  3        1  4  1  4  4   0.9   1.6   .04                                  EXAM0420
***** STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULTEXAM0430
  1   715        4        0        1        0      .20      .60      .70EXAM0440
  3                                 1        2                            EXAM0450
***** DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2 *****               EXAM0460
  1   712                                        .20      .35      .40EXAM0470
  3                                 3        4                            EXAM0480
***** DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4 *****                EXAM0490
  2   812                                                                  EXAM0500
  3        1  4  1  4  4   0.9   1.6   .04                                  EXAM0510
***** TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A EXAM0520
  3   906   155504   155503        0        0      .15        0      -.4EXAM0530
***** LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL *****    EXAM0540
  3   916   255504   155505        0        0      .15        0      -.4EXAM0550
***** LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL ***4EXAM0560
  3   902   555501        0        0      1.0      .25        0        0EXAM0570
                                  CUBANE                                   EXAM0580
  3  1102                                                                   EXAM0590
***** END OF SAVE SEQUENCE *****                                            EXAM0600
  3   202       9.                                                         EXAM0610
***** ADVANCE PLOTTER 9 INCHES ALONG X *****                                EXAM0620
  3   503        2     -2.7                                                EXAM0630
***** STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW *****     EXAM0640
  3  1103                                                                   EXAM0650
***** EXECUTE SAVED SEQUENCE FOR RIGHT EYE DRAWING *****                    EXAM0660
  3   202      20.                                                         EXAM0670
***** ADVANCE PLOTTER 20 INCHES *****                                       EXAM0680
  3   202                                                                  EXAM0690
***** ADD DUMMY PLOT TO MAGNETIC TAPE *****                                 EXAM0700
     -1                                                                    EXAM0710
```



CUBANE

Brookhaven Crystallographic Computer Program

NAME ØRTRAN FIELD 130 K_8 TIME <60 sec

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PRØGRAM ØRTRAN(INPUT,ØUTPUT,PUNCH,TAPE52,TAPE5=INPUT,
              TAPE6=ØUTPUT,TAPE7=PUNCH)
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ØRTRAN was written by W. R. Busing and W. E. Thiessen of Oak Ridge National Laboratory and installed at Brookhaven by G. J. B. Williams.

This program will search the reciprocal space of the normalized structure factors (E's) for the fourier transform of a known molecular fragment. The user may either search for the transform of a standard fragment, eg. a benzene ring, or define his own fragment and search for it. More than one orientation of the molecular fragment may be searched for and saved thus defining the orientation of repeated structural units.

If there are any comments or questions regarding the BNL version of this program these should be communicated to G. J. B. Williams.

****

DATA INPUT FOR ORTRAN APRIL, 1974

1) TITLE CARD

COLS
1-72 TITLE, ANY 72 CHARACTERS

2) CONTROL CARD

COLS
1- 3 ISTM, INDICATOR FOR STANDARD MOLECULAR FRAGMENT USED TO CALCULATE TRANSFORM.
0 - NON-STANDARD FRAGMENT, COORDINATES WILL BE READ.
NON-ZERO - STANDARD FRAGMENT CHOSEN AS FOLLOWS-

ISTM	FRAGMENT	LAUE GROUP	BOND LENGTH
1	BENZENE SKELETON	6/MMM	1.395*AD
2	CHAIR CYCLOHEXANE SKELETON	-3M	1.540*AD
3	ATOM PAIR	LINEAR	1.000*AD
4	CYCLOPROPANE SKELETON	6/MMM	1.514*AD

4- 6 NAT, NUMBER OF ATOMS USED TO GENERATE THE TRANSFORM. IF THE FRAGMENT IS CENTROSYMMETRIC THEN NAT IS HALF OF THE TOTAL NUMBER OF ATOMS. NAT IS SET BY THE PROGRAM IF ISTM IS NON-ZERO.

7- 9 INONC, INDICATOR FOR SYMMETRY OF FRAGMENT. SET BY THE PROGRAM IF ISTM IS NON-ZERO.
0 - CENTROSYMMETRIC
1 - NON-CENTROSYMMETRIC

10-12 IFC, INDICATOR FOR FRACTIONAL COORDINATES. SET BY THE PROGRAM IF ISTM IS NON-ZERO.
0 - ATOM COORDINATES IN CARTESIAN FORM
1 - ATOM COORDINATES REFERRED TO CRYSTAL AXES
RECOMMENDED INPUT IS 0 EXCEPT FOR SPECIAL PURPOSES SUCH AS COMPUTING THE VALUES OF THE TRANSFORM FOR A FRAGMENT FOUND IN AN E-MAP.

13-15 NS, NUMBER OF SYMMETRY CARDS (INCLUDING THE IDENTITY) NEEDED TO GENERATE A HEMISPHERE OF DATA. USUALLY FOR NON-CENTROSYMMETRIC CRYSTALS NS IS THE NUMBER OF EQUIVALENT POSITIONS. FOR CENTROSYMMETRIC CRYSTALS IT IS ONE HALF THIS NUMBER. FOR CENTERED CELLS, TRANSLATIONALLY EQUIVALENT POSITIONS NEED BE INCLUDED ONLY ONCE.

16-18 IBPS, INDICATOR TO BYPASS COARSE ROTATIONAL SEARCH
0 - PERFORM SEARCH
1 - BYPASS SEARCH AND READ NSV TRIAL ORIENTATIONS FOUND IN PREVIOUS SEARCH

19-21 NSV, NUMBER OF BEST ORIENTATIONS TO BE SAVED DURING COARSE SEARCH (OR TO BE READ IF IBPS = 1)

22-24 NRF, NUMBER OF BEST ORIENTATIONS TO BE USED AS STARTING POINTS FOR FINE SCANS AND/OR REFINEMENTS

25-27 MFS, FINE SCAN INDICATOR
0 - OMIT FINE SCAN
NON-ZERO - MAKE FINE SCANS AROUND NRF BEST

```
                ORIENTATIONS DIVIDING INTERVAL BY MFS. VALUES OF
                3 TO 5 MAY BE SUITABLE
28-30   NC, NUMBER OF CYCLES OF REFINEMENT TO BE MADE FOR EACH
            OF NRF STARTING POINTS. NC = 5 MAY BE SUITABLE
31-33   NPLOT, THE NUMBER OF BEST ORIENTATIONS FOR WHICH
            PRINTER PLOTS ARE TO BE MADE
34-36   KPLOT, INDICATOR FOR KIND OF PRINTER PLOT
            1 - GRID OMITTED. REFLECTIONS REPRESENTED AS FOLLOWS
                  *    E.GT.ELIM
                  0    E.LE.ELIM.AND.E.GT.ELIMF
                  +    E.LE.ELIMF
            2 - GRID INCLUDED. NUMBER OF SUPERIMPOSED
                REFLECTIONS PRINTED AT EACH POINT ON PLOT.
            3 - MAKE BOTH OF THE ABOVE KINDS OF PLOTS.
37-39   IVAX, CARTESIAN AXIS OF FRAGMENT DOWN WHICH
            PLOT IS VIEWED-
            1 FOR X-AXIS, 2 FOR Y-AXIS, 3 FOR Z-AXIS.
                USUAL VALUE IS 3
40-42   NLIST, THE NUMBER OF BEST ORIENTATIONS FOR WHICH LISTS
            OF DATA ARE TO BE MADE. THESE INCLUDE PLOTTER
            COORDINATES AND NS VALUES OF THE TRANSFORM
43-45   ILEQ, INDICATOR FOR LISTING EQUIVALENT REFLECTIONS
            0 - ONLY UNIQUE REFLECTIONS TO BE LISTED.
            1 - ENTIRE HEMISPHERE OF REFLECTIONS TO BE LISTED.
                RECOMMENDED VALUE IS 1
46-48   NPNCH, THE NUMBER OF BEST ORIENTATIONS FOR WHICH DATA
            CARDS ARE TO BE PUNCHED. THESE INCLUDE NS VALUES OF
            THE TRANSFORM
49-51   IPEQ, INDICATOR FOR PUNCHING EQUIVALENT REFLECTIONS
            0 - ONLY UNIQUE REFLECTIONS TO BE PUNCHED.
            1 - ENTIRE HEMISPHERE OF REFLECTIONS TO BE PUNCHED.
                RECOMMENDED VALUE IS 0
52-54   NOUT, DATA SET REFERENCE NUMBER FOR REFLECTION OUTPUT
            0 - PUNCHED CARDS
            NON-ZERO - AUXILIARY STORAGE ON DISK OR TAPE
55-57   IBPD, BYPASS INDICATOR FOR SYMMETRY CARDS AND DATA
            0 - READ SYMMETRY, DATA, AND TERMINATION CARDS
            1 - OMIT THESE CARDS (7), (8), AND (9) AND USE DATA
                READ ON PREVIOUS JOB
58-59   NOT USED
   60   KI(1) FOR P(1)    VARIABLE SELECTION INTEGERS FOR
   61   KI(2) FOR P(2)       REFINEMENT.
   62   KI(3) FOR P(3)       0 - PARAMETER FIXED
   63   KI(4) FOR AD         1 - PARAMETER TO BE VARIED
            USUALLY ALL FOUR PARAMETERS CAN BE VARIED, BUT
            IF FRAGMENT IS LINEAR ONE ANGLE P MUST BE FIXED.
            (USUALLY IT DOES NOT MATTER WHICH ONE IS FIXED.)

3) REAL CONSTANTS
   COLS
   1- 9 AD, OVERALL SCALE FACTOR TO BE APPLIED TO COORDINATES
            OF ATOMS IN FRAGMENT. SET AD = 1.0 FOR ISTM = 1, 2,
            OR 4. FOR ISTM = 3 SET AD EQUAL TO THE ATOM PAIR
            SEPARATION.
10-18   CHILIM, A SMALL ANGLE (DEGREES) USED TO TEST WHETHER
```

AN ORIENTATION IS SIGNIFICANTLY DIFFERENT FROM ONE FOUND PREVIOUSLY. A VALUE OF 1.0 MAY BE SUITABLE.

19-27 ELIM, THE MINIMUM ABSOLUTE VALUE OF E FOR REFLECTIONS TO BE INCLUDED IN THE COARSE ROTATIONAL SEARCH. USED TO SPEED UP SEARCH. DOES NOT AFFECT REFINEMENT. TRY A VALUE WHICH INCLUDES AT LEAST ONE HUNDRED STRONG REFLECTIONS IN THE HEMISPHERE.

28-36 ELIMF, SAME AS ELIM BUT USED FOR FINE SEARCH. MAKE ELIMF SMALLER THAN ELIM SO THAT MORE REFLECTIONS ARE INCLUDED IN THE FINE SCAN.

37-45 DAMPIN, DAMPING FACTOR APPLIED ON FIRST CYCLE OF REFINEMENT. INCREASED LINEARLY TO 1.0 ON CYCLE NC-1. A VALUE OF 0.5 IS A GOOD CHOICE. SET DAMPIN TO 1.0 FOR NO DAMPING

4) LATTICE PARAMETERS

COLS	
1- 9	A(1) = A (ANGSTROM UNITS)
10-18	A(2) = B
19-27	A(3) = C
28-36	A(4) = COS(ALPHA)
37-45	A(5) = COS(BETA)
46-54	A(6) = COS(GAMMA)

5) COORDINATES OF ATOMS USED TO GENERATE TRANSFORM. NAT CARDS. FOR CENTROSYMMETRIC MOIETIES INCLUDE ONLY ONE ATOM OF CENTROSYMMETRIC PAIR. FOR SYMMETRIC MOIETIES SUCH AS BENZENE THE HIGH ORDER AXIS SHOULD BE TAKEN ALONG Z. OMIT IF ISTM IS NON-ZERO.

COLS	
1- 9	NOT USED
10-18	F(J), THE SCATTERING FACTOR FOR ATOM J. IF F(J)=0 IT WILL BE RESET TO 1.0
19-27	NOT USED
28-36	XT(1,J) COORDINATES X, Y, Z OF ATOM IN FRAGMENT.
37-45	XT(2,J) CARTESIAN ANGSTROM UNITS IF IFC=0,
46-54	XT(3,J) FRACTIONAL CRYSTAL UNITS IF IFC=1.
	THESE WILL BE MULTIPLIED BY AD

6) DESCRIPTION OF COARSE LATTMAN SCAN. THIS CARD MUST ALWAYS BE INCLUDED. IF I8PS=1 INDICATING THAT NO COARSE SCAN IS TO BE MADE THE INPUT WILL BE NEEDED TO SET UP ANY DESIRED FINE SCANS

COLS	
1- 3	ILS, LATTMAN SCAN LIMIT INDICATOR

0 - LIMITS ARE TO BE READ FROM THIS CARD

NON-ZERO - STANDARD LIMITS ARE TO BE TAKEN FROM DATA IN ARRAYS WDT AND LDT AS FOLLOWS -

ILS	LAUE GROUP OF MOIETY	UNIQUE AXIS	LAUE GROUP OF CRYSTAL	UNIQUE AXIS
1	-1	-	-1	-
2	2/M	Z	-1	-
3	MMM	-	-1	-
4	-3	Z	-1	-
5	-3M	Z	-1	-

6	6/M	Z	-1	-
7	6/MMM	Z	-1	-
8	LINEAR	Z	-1	-
11	-1	-	2/M	B
12	2/M	Z	2/M	B
13	MMM	-	2/M	B
14	-3	Z	2/M	B
15	-3M	Z	2/M	B
16	6/M	Z	2/M	B
17	6/MMM	Z	2/M	B
18	LINEAR	Z	2/M	B
21	-1	-	MMM	-
22	2/M	Z	MMM	-
23	MMM	-	MMM	-
24	-3	Z	MMM	-
25	-3M	Z	MMM	-
26	6/M	Z	MMM	-
27	6/MMM	Z	MMM	-
28	LINEAR	Z	MMM	-
31	-1	-	2/M	C
32	2/M	Z	2/M	C
33	MMM	-	2/M	C
34	-3	Z	2/M	C
35	-3M	Z	2/M	C
36	6/M	Z	2/M	C
37	6/MMM	Z	2/M	C
38	LINEAR	Z	2/M	C

IT IS ALWAYS PERMISSIBLE TO USE LIMITS APPROPRIATE TO SUB-GROUPS OF THE ACTUAL SYMMETRIES OF THE FRAGMENT OR CRYSTAL. THIS WILL INCREASE THE TIME REQUIRED FOR THE COARSE SCAN, AND SEVERAL EQUIVALENT ORIENTATIONS WILL BE FOUND, BUT IT SHOULD CAUSE NO OTHER DIFFICULTY.

IF ILS IS NON-ZERO THEN THE REMAINDER OF THIS CARD, EXCEPT FOR W2D, MAY BE LEFT BLANK.

4	L2I, 0 IF LIMIT W2I IS NOT INCLUDED IN SCAN, 1 IF IT IS
5	L2F, 0 IF LIMIT W2F IS NOT INCLUDED IN SCAN, 1 IF IT IS
6	LPI, 0 IF LIMIT WPI IS NOT INCLUDED IN SCAN, 1 IF IT IS
7	LPF, 0 IF LIMIT WPF IS NOT INCLUDED IN SCAN, 1 IF IT IS
8	LMI, 0 IF LIMIT WMI IS NOT INCLUDED IN SCAN, 1 IF IT IS
9	LMF, 0 IF LIMIT WMF IS NOT INCLUDED IN SCAN, 1 IF IT IS
10-18	W2D, INCREMENT (DEGREES) FOR LATTMAN THETA TWO. DO NOT OMIT. A VALUE OF 10.0 IS USUALLY SUITABLE.
19-27	W2I, INITIAL VALUE (DEGREES) FOR LATTMAN THETA TWO
28-36	W2F, FINAL VALUE (DEGREES) FOR LATTMAN THETA TWO
37-45	WPI, INITIAL VALUE (DEGREES) FOR LATTMAN THETA PLUS
46-54	WPF, FINAL VALUE (DEGREES) FOR LATTMAN THETA PLUS. WPF MUST BE GREATER THAN (NOT EQUAL TO) WPI
55-63	WMI, INITIAL VALUE (DEGREES) FOR LATTMAN THETA MINUS. WMF MUST BE GREATER THAN (NOT EQUAL TO) WMI
64-72	WMF, FINAL VALUE (DEGREES) FOR LATTMAN THETA MINUS

7) SYMMETRY INFORMATION USED TO EXPAND DATA SET TO FULL HEMISPHERE. NS CARDS EACH OF WHICH DESCRIBES ONE SYMMETRY OPERATION ARE READ. INCLUDE THE BASIC POSITION X, Y, Z. INCLUDE ONLY ONE OF A CENTROSYMMETRICALLY RELATED PAIR. FOR CENTERED CELLS, TRANSLATIONALLY EQUIVALENT POSITIONS NEED BE INCLUDED ONLY ONCE.
OMIT THESE CARDS IF IBPD=1.

TRANSFORMED COORDINATES WOULD BE IN THE FORM

```
X(NEW)=T(X)+M(XX)*X+M(XY)*Y+M(XZ)*Z
Y(NEW)=T(Y)+M(YX)*X+M(YY)*Y+M(YZ)*Z
Z(NEW)=T(Z)+M(ZX)*X+M(ZY)*Y+M(ZZ)*Z
```

TRANSFORMED INDICES ARE

```
H(NEW)=M(XX)*H+M(YX)*K+M(ZX)*L
K(NEW)=M(XY)*H+M(YY)*K+M(ZY)*L
L(NEW)=M(XZ)*H+M(YZ)*K+M(ZZ)*L
```

COLS	
1-15	T(X)
16-18	M(XX)
19-21	M(XY)
22-24	M(XZ)
25-39	T(Y)
40-42	M(YX)
43-45	M(YY)
46-48	M(YZ)
49-63	T(Z)
64-66	M(ZX)
67-69	M(ZY)
70-72	M(ZZ)

8) REFLECTION DATA CARDS. OMIT IF IBPD = 1. OTHERWISE INCLUDE THOSE WITH E GREATER THAN SOME LIMIT SUCH AS 1.5, FOR EXAMPLE. THE FORMAT CAN BE CHANGED BY MODIFYING SUBROUTINE OBSIN. THE STANDARD FORMAT IS AS FOLLOWS-

COLS	
1	ISENT, BLANK OR ZERO
2- 4	H(1), THE INDEX H
5- 8	H(2), THE INDEX K
9-12	H(3), THE INDEX L
13-21	E, THE NORMALIZED STRUCTURE FACTOR (SIGNED OR UNSIGNED)

9) REFLECTION DATA TERMINATION CARD. OMIT IF IBPD=1

COLS	
1	ISENT=1

10) ANGLES FOR TRIAL ORIENTATIONS FOUND IN PREVIOUS SEARCH. INCLUDE NSV CARDS ONLY IF IBPS=1. THESE WILL BE USED AS STARTING POINTS FOR FINE SCANS AND/OR REFINEMENTS

COLS	
1- 9	W1, THE EULER ANGLE THETA ONE (DEGREES)
10-18	W2, THE EULER ANGLE THETA TWO (DEGREES)
19-27	W3, THE EULER ANGLE THETA THREE (DEGREES)

```
11) REPEAT INPUTS (1) TO (10) AS MANY TIMES AS DESIRED
*****************************************************************
RETURN
END
```

Brookhaven Crystallographic Computer Programs

NAME: PØWPAT

CØRE: 135 K

PRØGRAM PØWPAT(INPUT,ØUTPUT)

I. Purpose: To calculate the intensities of powder patterns obtained in X-ray or neutron diffraction experiments.

II. Tapes: None

III. Limitations: 8 atom types

IV. Replaceable Subroutines: None

V. Deck Setup

A. Job Card

1. Time limit - less than 77
2. Field length - 135 K
3. Line limit -
4. Number of tapes- 0
5. ECS - 0

B. Control Cards

```
ATTACH(PØWPAT,PØWPAT,ID=CPRØGS)
PØWPAT.
```

A FORTRAN IV PROGRAM FOR THE INTENSITY CALCULATION OF POWDER PATTERNS

(1969 Version)

by

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Abstract

This report describes a revised edition of a computer program written in Fortran IV language to calculate the intensities of powder patterns obtained in X-ray or neutron diffraction experiments. The program has run successfully on the IBM 360 computer at the University of Pennsylvania Computer Center. The report contains a copy of the print-out of the program and instructions for the use of this program, illustrated with actual examples.

The original program was written in 1966 in connection with crystal structure studies supported by U. S. Public Health Service Research Grant DE-02135 from the National Institute of Dental Research and the Advanced Research Projects Agency of the Department of Defense Contract SD-69. The financial support of the sponsoring agency is gratefully acknowledged.

NOTE: A limited number of card decks may be obtained by writing to the authors. Anyone using this program does so at his own risk. We appreciate any comments to improve or, if necessary, correct this program.

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A. The Physical Background.

a) The position of the diffraction lines on a powder pattern can be obtained from the Bragg Law: $\sin^2\theta_{hk\ell} = \lambda^2/4d^2_{hk\ell}$

Inserting the proper equations for $d_{hk\ell}$ one obtains the following equations for the different crystal systems (input variable ISYSTM):

Cubic system: $$\sin^2\theta_{hk\ell} = \frac{\lambda^2}{4a^2}(h^2+k^2+\ell^2)$$

(ISYSTM = 5)

Tetragonal system: $$\sin^2\theta_{hk\ell} = \frac{\lambda^2}{4a^2}(h^2+k^2)+\frac{\lambda^2}{4c^2}\ell^2$$

(ISYSTM = 4)

Hexagonal and trigonal (hexagonal lattice) system: $$\sin^2\theta_{hk\ell} = \frac{\lambda^2}{3a^2}(h^2+hk+k^2)+\frac{\lambda^2}{4c^2}\ell^2$$

(ISYSTM = 6 or 3)
see page 11

Orthorhombic system: $$\sin^2\theta_{hk\ell} = \frac{\lambda^2}{4a^2}h^2+\frac{\lambda^2}{4b^2}k^2+\frac{\lambda^2}{4c^2}\ell^2$$

(ISYSTM = 2)

Monoclinic system: (old setting, $\beta \neq 90°$) $$\sin^2\theta_{hk\ell} = \frac{\lambda^2}{4a^2\sin^2\beta}h^2+\frac{\lambda^2}{4b^2}k^2+\frac{\lambda^2}{4c^2\sin^2\beta}\ell^2-\frac{\lambda^2\cos\beta}{2ac\sin^2\beta}h\ell$$

(ISYSTM = 1)

Triclinic system: $$\sin^2\theta_{hk\ell} = \frac{\lambda^2}{4}\Big[h^2\left(\frac{bc\sin\alpha}{V}\right)^2+k^2\left(\frac{ca\sin\beta}{V}\right)^2+\ell^2\left(\frac{ab\sin\gamma}{V}\right)^2+$$

(ISYSTM = 7)

$$+2k\ell\frac{a^2bc}{V^2}\left(\cos\beta.\cos\gamma-\cos\alpha\right)+2\ell h\frac{ab^2c}{V^2}\left(\cos\gamma.\cos\alpha-\cos\beta\right)+$$

$$+2hk\frac{abc^2}{V^2}\left(\cos\alpha.\cos\beta-\cos\gamma\right)\Big]$$

where $$V = 2abc\sqrt{\sin\frac{\alpha+\beta+\gamma}{2}.\sin\frac{-\alpha+\beta+\gamma}{2}.\sin\frac{\alpha-\beta+\gamma}{2}.\sin\frac{\alpha+\beta-\gamma}{2}}$$

The program provides the $hk\ell$, $\sin^2\theta$, θ and d values of all possible reflections in the order of increasing θ or $\sin^2\theta$ values. All those $hk\ell$ which are not allowed due to the symmetry of the space group (control variables IBRAVL, IHKO, IOKL, IHOL, IHHL, IHOO, IOKO and IOOL) will not be calculated. Maximum number of $\sin^2\theta$ is 3000.

b) The intensity of the diffraction line of a powder pattern is given by

$$I_{hk\ell} = m.\ LP.\ A.\left[\sum_{j}^{\text{unit cell}} f_j.\ O_j.\ e^{-B_j.\frac{\sin^2\theta}{\lambda^2}}\ .\ e^{2\pi i(hx_j + ky_j + \ell z_j)}\right]^2$$

where

m	multiplicity factor
LP	Lorentz-Polarization factor
A	absorption factor
B_j	isotropic temperature coefficient of atom j
f_j	atomic scattering factor of atom j
O_j	occupation factor of site xyz with atom j

The program in the calculations of intensities does not use any symmetry relationship between the point positions except for the special cases that the structure contains a symmetry center at the origin and/or is based on a non-primitive Bravais lattice.

b1) The multiplicity factors are included in the program with values as given in Table 3.5.1 of Vol. 1 of the International Tables for x-ray Crystallography. All systems with higher than 2-fold symmetry have

a high-symmetry and a low-symmetry Laue group. Some of the forms in the lower-symmetry Laue group have the same spacing, but their intensities of reflection are different. They will give rise to the same line in a powder photograph, but the intensity of the line will be due to the sum of the reflections from the two forms. It is therefore necessary to distinguish in the program between high- and low-symmetry Laue groups by proper choice of the input variable LAUE. In the calculation of structures with trigonal symmetry (hexagonal cell), the hkℓ - values and the multiplicity factors will be taken as corresponding to the low-Laue symmetry case. Therefore for trigonal structures with high Laue symmetry certain reflections will be listed separately in the output list although they have the same d spacing and same intensity.

In order to check the intensity calculation, the multiplicity factor used is printed on the same line of each intensity value for all cases.

b2) <u>The Lorentz-Polarization factor.</u> The program permits five different LP-factors to be used. The particular Lorentz-Polarization formula is determined by the value of the input variable KODLP.

For x-rays the LP-factor amounts to

$$LP_{x\text{-rays}} = \frac{1 + \cos^2 2\theta}{\sin^2 \theta . \cos \theta} \qquad KODLP = 0$$

For some calculations, the LP-factor may be given unity

$$LP_{special} = 1 \qquad KODLP = 1$$

For neutron-diffraction, the polarization part drops out and one obtains

$$LP_{neutrons} = \frac{1}{\sin^2\theta . \cos\theta} \qquad KODLP = 2$$

The intensity calculation for powder patterns of diffractometer experiments using a monochromator requires a LP-factor which is dependent on the diffraction angle 2α in the monochromator. (Input variable for 2α: AGUIN)

$$LP_{monochromator} = \frac{(1 + \cos^2 2\alpha . \cos^2 2\theta)}{\sin^2\theta . \cos\theta} \qquad KODLP = 3$$

For the interpretation of powder patterns recorded with the GUINIER-DE WOLFF focussing camera the following LP-correction will be used:

$$LP_{Guinier} = \frac{1 + \cos^2 2\alpha . \cos^2 2\theta}{\sin\theta . \cos^2(2\theta - \beta) . \sin 2\theta} \qquad KODLP = 4$$

2α = diffraction angle in monochromator (input variable for 2α: AGUIN)

β = angle between the incoming beam and the normal to the plane of the specimen (input variable: BGUIN)

b3) <u>The absorption factor A</u> depends on the experimental set-up. For flatplate diffractometer experiments the absorption factor is a constant. For cylindrical specimens in a Debye-Scherrer camera the absorption

factor is a function of θ. The exact calculation of A is difficult. Therefore no absorption correction has been provided in the program.

b4) Atom positions: Up to eight different kinds of atoms are permitted in the program (max. value of NCOMPO is eight). It is to be understood that atoms are of the same kind if they have the same atomic scattering factor. For each different kind of atom there can be 48 different data cards with point positions which may be from different equipoints. Except for the special cases where the structure contains a symmetry center at the origin and/or has a non-primitive Bravais lattice all point positions per unit cell have to be listed on data cards.

For the case of a non-primitive Bravais lattice only the non-translation related point positions have to be included in the input. If the proper IBRAVL value has been entered the intensities will be multiplied by the appropriate factor. Reflections which are forbidden according to the proper Bravais lattice extinction law will not appear in the final output.

If one wants to take advantage of a symmetry center at the origin to reduce the data input by one-half one must use the input variables ISYMCE and FOCCU (M). With ISYMCE = 1 the sine part of the structure factor is set to zero. The atom occupation factor FOCCU(M) is normally set at 1, however, for the intensity calculations of defect and disorder structures the factor can be made smaller. Whatever value is used for the atom occupation factor, disregarding the symmetry center, it has to be doubled if the data input is to be reduced by one-half due to the center of symmetry at the origin. In other words, for all those

atom positions xyz which have a symmetry related mate $\bar{x}\bar{y}\bar{z}$ only the xyz values have to be listed in the data cards provided that the occupation factor FOCCU (M) for those atoms is increased to twice its value (thus FOCCU (M) = 2 for non-defect structures). However, atoms which are located at symmetry centers, for example at 000, $\frac{1}{2}$ 0 0, 0 $\frac{1}{2}$ 0, 0 0 $\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}$ 0, $\frac{1}{2}$ 0 $\frac{1}{2}$, 0 $\frac{1}{2}\frac{1}{2}$ or $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, are their own symmetry mates and the occupation factors for those atoms must have the non-doubled values of FOCCU (M).

b5) <u>The isotropic temperature-factor</u> is of the form $e^{-(B.\sin^2\theta)/\lambda^2}$ where B is the Debye-Waller temperature coefficient (input variable BTEMP) to be used for each kind of atom.

b6) <u>The atomic scattering factor</u> in the case of x-rays is a function of $\sin\theta/\lambda$ and will be described depending on the input variable ISCAT <u>either</u> by an exponential function of the type

$$f_{x\text{-}ray} = A.\ e^{-a\left(\frac{\sin^2\theta}{\lambda^2}\right)} + B.\ e^{-b\left(\frac{\sin^2\theta}{\lambda^2}\right)} + C \quad \text{(ISCAT = 0)}$$

with constants given by F. H. Moore: Acta Cryst. <u>16</u> 1169 (1963). (a copy of Moore's tables can be found in the appendix.)

<u>or</u> by a linear interpolation of 30 different form factor values for increasing $\frac{\sin\theta}{\lambda}$ ratios listed in the International Tables for X-ray Crystallography, Vol. III, Table 3.3.1. (ISCAT = 1)

In the case of neutron diffraction the scattering amplitude is independent of $\frac{\sin\theta}{\lambda}$. One has to use the exponential function with all constants except C equal to zero. The value to be inserted is tabulated in the International Tables for X-ray Crystallography, Vol. III, Table 3.3.4A. For details see page 13. (ISCAT = 0)

Under certain conditions the anomalous dispersion must be considered. The atomic scattering factor is then given by

$$f_{total} = f\left(\frac{\sin\theta}{\lambda}\right) + \Delta f' + i\Delta f''$$

where $\Delta f'$ and $\Delta f''$ may be taken from Tables 3.3.2A, B and C in the Int. Tables, Vol. III. Friedel's law does not hold anymore and the values of $|F_{hk\ell}|^2$ and $|F_{\bar{h}\bar{k}\bar{\ell}}|^2$ are now given by

$$|F_{hk\ell}|^2 = (A' - B'')^2 + (B' + A'')^2 \text{ and}$$

$$|F_{\bar{h}\bar{k}\bar{\ell}}|^2 = (A' + B'')^2 + (B' - A'')^2$$

$$\text{where } A' = \sum_{j}^{\text{unit cell}} \left(f_j\left(\frac{\sin\theta}{\lambda}\right) + \Delta f_j'\right) \cos 2\pi\left(hx_j + ky_j + \ell z_j\right)$$

$$A'' = \sum_{j}^{\text{unit cell}} \Delta f_j'' \cos 2\pi\,(hx_j + ky_j + \ell z_j)$$

and B' and B'' the corresponding sine summations. The structure factor square for a powder line can be calculated to

$$|F|^2 = \frac{|F_{hk\ell}|^2 + |F_{\bar{h}\bar{k}\bar{l}}|^2}{2} = \underbrace{(A')^2 + (B')^2}_{|F'|^2} + \underbrace{(A'')^2 + (B'')^2}_{|F''|^2}$$

No particular provisions have been made in the program to calculate the total powder intensities for the case of anomalous dispersion. However $|F'|^2$ can be obtained simply <u>either</u> by adding the value of $\Delta f'$ to the C variable in Moore's approximation (CCC(M) on card 5; ISCAT = 0) <u>or</u> by adding the value of $\Delta f'$ to each of the 30 different form factor values (SFA(I, M) on card 6 and 7; ISCAT = 1). A list of the additive corrections $|F''|^2$ can be obtained by running the program separately with only $\Delta f''$ inserted for the C constant of Moore's approximation.

First data card: Number of problems to be calculated Format (I2)

NCALCS: This is the very first data card and defines the number of problem sets which follow.

The input data for <u>each</u> problem set is outlined in pages 9-15.

B. Description of data cards for each problem

Note - See previous page

First data card: (Title) Format (20A4)

COMPND:	All eighty columns can be used for title and description, which will be printed unchanged as first line of the output.

Second data card: (Unit cell data) Format (6F10.0)

A, B, C:	Lattice parameters in Ångström. b and c can be omitted for cubic unit cell; b can be omitted for tetragonal or hexagonal unit cell.
ALPHA, BETA, GAMMA:	Unit cell angles in degrees to be given only for triclinic (also for rhombohedral cells which must be calculated as triclinic) and monoclinic unit cells. In the monoclinic case, the old setting with the 2 fold axis taken as the y-axis must be used (α, $\gamma = 90°$). In this case α and γ can be omitted. The setting with $\alpha = \beta = 90° \neq \gamma$ must be calculated as triclinic cell.

Third data card: (Experimental set-up) Format (F10.0, 2F5.0, 4I2, 2X, 2F10.0)

WL:	Wavelength in Ångström
SL: SH:	lowest highest } $\sin^2\theta$ value, which will be included in the calculation, SL value may be zero; if no value is given for SH, the maximum $\sin^2\theta$ value will be set to 0.999.

NORM: Option allowing different output features (see section C)

Output ~~A~~ B (0)

Output ~~B~~ A (1) (normal case)

ISCAT: Indicates whether constants for exponential function describing the atomic scattering factor or form factor tables are used. Constants of exponential function AAA (M), AA (M), BBB (M), BB (M), CCC (M) on fifth data card are used: ISCAT = 0. Scattering factor values from tables (SFA (I, M), I = 1, 30) are used: ISCAT = 1

Note: If ISCAT = 0, data cards "6" and "7" must be omitted.

If ISCAT = 1, two cards with form factor tables must follow each card "5".

IMAGE: Graphic representation of intensity output wanted.

Yes (1)

No (0)

KODLP: Lorentz-Polarization factor to be used.

X-rays	(0)
LP = 1	(1)
Neutrons	(2)
Monochromator	(3)
GUINIER	(4)

See Appendix G for neutron Scattering Amplitudes

AGUIN: For the calculation of the LP-factor in diffraction experiments using a monochromator. AGUIN = value of the diffraction angle 2α in degrees. Must be used only if KODLP = 3 or 4.

BGUIN: For Guinier experiments; BGUIN = angle (in degrees) between the incoming beam and the perpendicular to the plane of the specimen; must be used only if KODLP = 4.

Fourth data card: (Structure type data) Format (4I2, 2X, 7I2, 6X, 9I2)

ISYSTM: Code word defining the crystal system; monoclinic (1), orthorhombic (2), trigonal (3), tetragonal (4), cubic (5) hexagonal (6), triclinic (7). For rhombohedral see below.

IBRAVL: Indicator for Bravais-Lattice type:

P(1) primitive

I(2) I-centered $+[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

R(3) rhombohedral obverse $(-h+k+\ell = 3n)$

$+[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}; \frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$

F(4) F - centered $+[\frac{1}{2}, \frac{1}{2}, 0; 0, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, 0, \frac{1}{2}]$

A(5) A-centered $+[0, \frac{1}{2}, \frac{1}{2}]$

B(6) B-centered $+[\frac{1}{2}, 0, \frac{1}{2}]$

C(7) C-centered $+[\frac{1}{2}, \frac{1}{2}, 0]$

IBRAVL = 3 refers to the obverse setting only.

Attention must be paid to the proper use of the variables, ISYSTM and IBRAVL in the trigonal case. For P-space groups ISYSTM = 3 and IBRAVL = $\overset{1}{0}$ will be used. All $hk\ell$ values will be calculated. For R - space groups, there are two possibilities: If the structure is described with

the triple hexagonal cell, ISYSTM = 3 and IBRAVL = 3 have to be used. Consequently, all $hk\ell$ values with $-h+k+\ell \neq 3n$ will not appear in the output. If a structure of space group R must be described with a rhombohedral unit cell, ISYSTM = 7 and IBRAVL = $\overset{1}{0}$ have to be used. This corresponds to a triclinic description of the unit cell and therefore the angles α, β and γ must not be omitted in the input ($\alpha = \beta = \gamma$). Also a number of reflections which actually coincide are calculated separately and appear as such in the output.

LAUE: Code word defining the Laue symmetry. See also page 4.

Low L.S. (1)

High L.S. (2)

ISYMCE: Center of symmetry at origin. See page 6.

Yes (1)

No (0)

IHKO: Conditions for possible hk0 reflections

(1)	No restriction	(2)	$h+k = 2n$ only
(3)	$k = 2n$ only	(4)	$h+k = 4n$ only
(5)	$h = 2n$ only		

IOKL: Conditions for possible $0k\ell$ reflections

(1)	No restriction	(2)	$k+\ell = 2n$ only
(3)	$\ell = 2n$ only	(4)	$k+\ell = 4n$ only
(5)	$k = 2n$ only		

IHOL: Conditions for possible $h0\ell$ reflections

(1)	No restriction	(2)	$h+\ell = 2n$ only
(3)	$\ell = 2n$ only	(4)	$h+\ell = 4n$ only
(5)	$h = 2n$ only		

IHHL: Conditions for possible hhℓ reflections

(1) No restriction	(2) ℓ = 2n only
(3) 2h + ℓ = 4n only	

IHOO: Conditions for possible h00 reflections

(1) No restriction	(2) h = 2n only
	(4) h = 4n only

IOKO: Conditions for possible 0k0 reflections

(1) No restriction	(2) k = 2n only

IOOL: Conditions for possible 00ℓ reflections

(1) No restriction	(2) ℓ = 2n only
(3) ℓ = 3n only	(4) ℓ = 4n only
	(6) ℓ = 6n only

NCOMPO: Number of different kinds of atoms in compound. The maximum number is eight.

NA(M): Number of data cards with point positions for atoms of kind M. This number corresponds to the number of atoms of kind M per unit cell if the Bravais lattice factor IBRAVL is set for a primitive Bravais lattice. NA(M) is a quarter or a third or one-half of the number of atoms of kind M per unit cell depending if the structure is based on a face centered, triple-hexagonal or body and side centered Bravais lattice.

Fifth data card: (Scattering factor) Format (A4, F6. 0, 6F10. 0)

ELEMT(M): Chemical symbol of element M (Alphanumeric Information

FOCCU(M): Occupation factor for centrosymmetric and defect structures. If left blank, the occupation factor is automatically set to 1.0.

AAA(M), AA(M), BBB(M), BB(M), CCC(M): The five constants A, a, B, b and C for the exponential approximation of the x-ray scattering factor after F. H. Moore: Acta Cryst. 16, 1169(1963) (See appendix). For neutron diffraction the fields for AAA(M), AA(M), BBB(M), BB(M) have to be left blank and the neutron scattering coefficient is to be inserted, together with its sign, in place of CCC(M). If ISCAT = 1, no values for the 5 constants are necessary.

BTEMP(M): Temperature factor coefficient. If left blank, no temperature correction will be made.

Sixth Data Card: and Seventh Data Card:

Format (5X, 15F5.0)
Format (15F5.0)
} Optional, only if ISCAT = 1

SFA(I, M): Scattering factor tables. These two cards are to be included only when ISCAT = 1 on the 3rd data card. There are 2 cards for each table. Each card contains 15 values of the atomic form factor at intervals of $\sin \theta/\lambda = 0.05$, starting at $\sin \theta/\lambda = 0$.

Sixth Card: Columns

1-5:	May be left blank. Can be used to identify card.	
6-10:	form factor for $\sin \theta/\lambda = 0.00$	SFA(1, M)
11-15:	" " " " " $= 0.05$	SFA(2, M)
16-20:	" " " " " $= 0.10$	SFA(3, M)
⋮	⋮	⋮
76-80:	" " " " " $= 0.70$	SFA(15, M)

Seventh Card: Columns

1-5:	" " " " " $= 0.75$	SFA(16, M)
⋮	⋮	⋮
71-75:	" " " " " $= 1.45$	SFA(30, M)
76-80:	May be left blank; can be used to identify card.	

These factors may be found in: Int. Tables Vol. III, Table 3.3.1. Atomic form factors for $\frac{\sin \theta}{\lambda}$ values between those given in the table above will be calculated by linear interpolation.

<u>Eighth data card:</u> (Atom positions) Format (3F10.0)

This card is the eighth data card if ISCAT = 1 or actually the sixth data card if ISCAT = 0

X(I, M), Y(I, M), Z(I, M): Point positions of the ith atom of kind M. There can be a maximum of 48 point position data for each of the eight different kinds of atoms. The number of type "eight" cards is equal to NA(M).

Another type "five" card follows if the structure contains another kind of atom. Other cards of type "six" (optional), "seven" (optional), and "eight" must follow containing the point positions of the new kind of atoms.

C. The Output

The first part of output is a print-out of the input data in a more readable format.

The second part is controlled by the input variable NORM and lists in the order of increasing $\sin^2\theta$ the calculated values of $hk\ell$, θ, 2θ, d(Å), $\sin\theta$, $\sin^2\theta \cdot 10^3$, $hk\ell$, intensity (normalized to a scale of 1000), $/F(hk\ell)/^2$, real and imaginary components of structure-factors followed on the same line by the phase angle, multiplicity factor and the LP-factor used (Output A corresponding to input variable NORM = 1). However, for unit cells or intensity calculations providing very large structure factors or having more than 3000 ($hk\ell$) - values, it is desirable not to normalize the intensity which can be done by giving NORM the valu zero. The following values will be printed out: $hk\ell$, θ, $\sin^2\theta$, scaled intensity, unscaled intensity, $/F(hk\ell)/^2$, real and imaginary part of structure factor, phase angle, multiplicity factor, LP-factor (Output B corresponding to NORM = 0). The calculation range is governed by the input variables SL and SH, which set the lowest and highest $\sin^2\theta$ values respectively.

The third part of the output is obtained only if the input variable IMAGE is entered with the value 1. It is a graphical presentation of the diffraction pattern using rows of asteriks proportional to the intensities in steps of one-half degree θ. If more than one line occurs within the half-degree range, their intensities are added.

The complete diffraction pattern is rescaled to hundred asteriks for the strongest line.

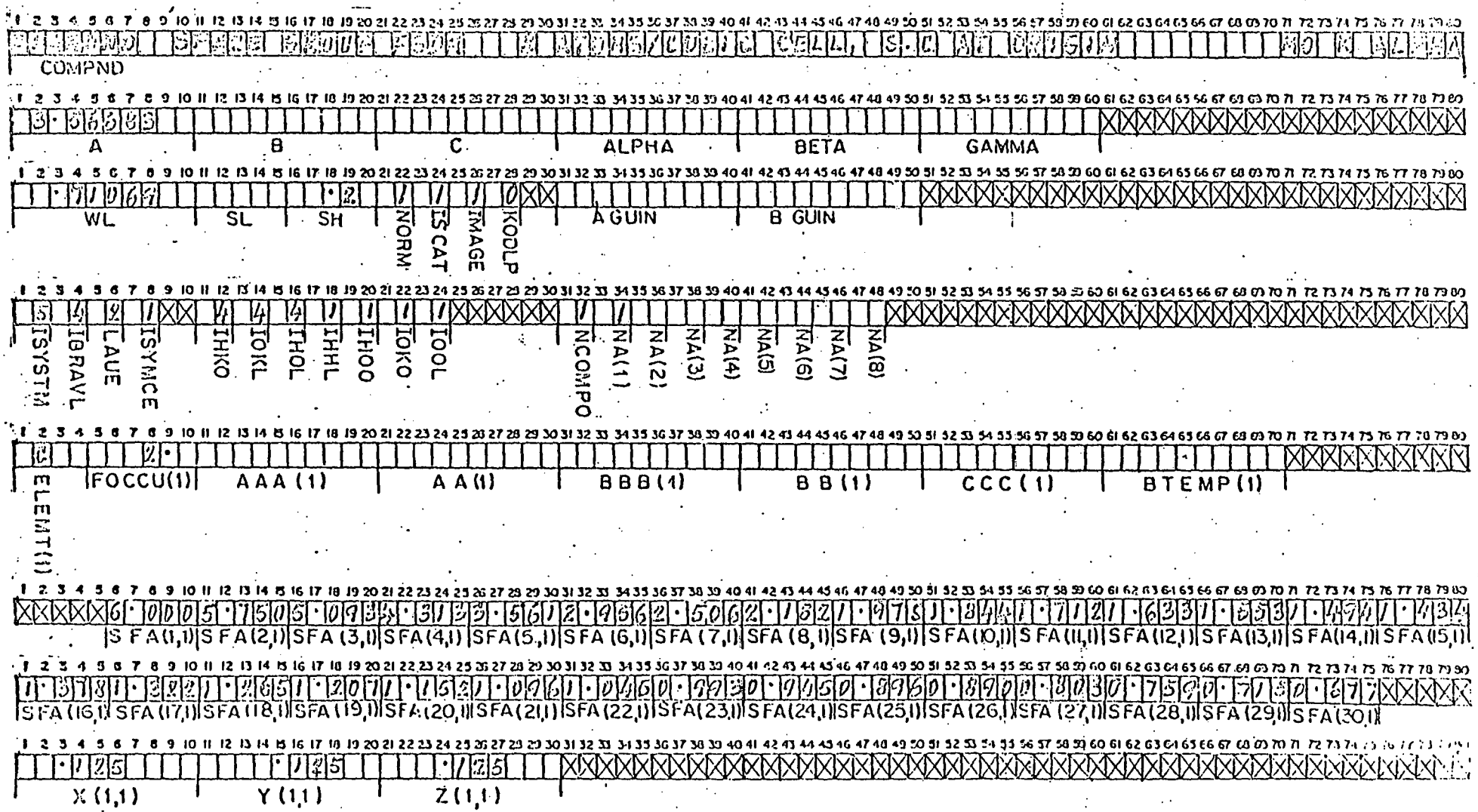
In certain instances the program might be used for the interpretation of single crystal diffraction data. In this case it is desirable to suppress the ordering of the hkl values with increasing $\sin^2\theta$ values. This can be done easily by inserting a "GO TO 80" statement after YJP 387. In the output the hkl values will then appear in the order they were generated. For this calculation it is necessary to give the variable "IMAGE" the value 0.

Running time:

The running time for most powder patterns is less than a minute.

D. Input and output examples

1st Example: X-diffraction pattern of diamond. Cubic cell with symmetry center at origin. Output A. Scattering factor tables are used. All crossed-out blocks will not be read by the computer and may be used to characterize data card.



```
INTENSITY CALCULATION FOR DIAMOND  SPACE GROUP F3DM   8 ATOMS/CUBIC CELL, S.C. AT ORIGIN        MO K ALPHA

DATA CALCULATED FOR A CUBIC STRUCTURE WITH
A=  3.56683,WL= 0.71069 ANGSTROM
 SIN-SQUARE-THETA-VALUES CALCULATED BETWEEN SL= 0.0    AND SH= 0.2000          KOOLP= 0          AGUIN= 0.0        BGUIN= 0.0
DATA CALCULATED FOR HIGH LAUE-SYMMETRY
FACECENTERED BRAVAISLATTICE,H,K,L ALL EVEN OR ALL ODD
HKO ONLY WITH H+K=4N
OKL ONLY WITH K+L=4N
HOL ONLY WITH H+L=4N
SYMMETRY CENTER AT ORIGIN OF UNIT CELL
            ATOMS IN UNIT CELL: ELEMT(M)  NA(M)*NBRA*FOCCU(M)
                                  C        1  * 4  *  2.00

SCATTERING FACTORS OF C    IN STEPS OF .05*SIN(THETA)/LAMBDA
 6.000  5.750  5.093  4.313  3.561  2.956  2.506  2.182  1.975  1.844  1.712  1.633  1.553  1.494  1.434
 1.378  1.322  1.265  1.207  1.152  1.096  1.045  0.993  0.945  0.896  0.850  0.803  0.759  0.715  0.677

BTEMP=   0.0      ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS    2.00000

C        0.12500   0.12500   0.12500   +(1/2 1/2 0,1/2 0 1/2,0 1/2 1/2)
```

H	K	L	THETA	2THETA	D-VALUE	SIN	SIN2*1000	H	K	L	INTENSITY	/F(HKL)/**2	A(HKL)	B(HKL)	PHA.ANG.	MULT	LPG
1	1	1	9.94	19.87	2.0593	0.1726	29.78	1	1	1	1000.0	296.3	-17.21	0.0	180.000	8.	64.25
2	2	0	16.37	32.73	1.2611	0.2818	79.40	2	2	0	447.3	253.3	-15.92	0.0	180.000	12.	22.41
3	1	1	19.29	38.59	1.0754	0.3304	109.18	3	1	1	256.7	104.2	-10.21	0.0	180.000	24.	15.53
2	2	2	20.19	40.38	1.0297	0.3451	119.10	2	2	2	0.0	0.0	-0.00	0.0	180.000	8.	14.14
4	0	0	23.48	46.97	0.8917	0.3985	158.80	4	0	0	66.2	167.1	-12.93	0.0	180.000	6.	10.06
3	3	1	25.74	51.48	0.8183	0.4343	188.58	3	3	1	97.7	75.9	8.71	0.0	0.0	24.	8.17

DIFFRACTION PATTERN FOR DIAMOND SPACE GROUP F3DM 8 ATOMS/CUBIC CELL, S.C. AT ORIGIN MO K ALPHA WL= 0.71069

```
 0.0
 0.5
 1.0
 1.5
 2.0
 2.5
 3.0
 3.5
 4.0
 4.5
 5.0
 5.5
 6.0
 6.5
 7.0
 7.5
 8.0
 8.5
 9.0
 9.5   ****************************************************************************************************
10.0
10.5
11.0
11.5
12.0
12.5
13.0
13.5
14.0
14.5
15.0
15.5
16.0   *********************************************
16.5
17.0
17.5
18.0
18.5
19.0   ****************************
19.5
20.0
20.5
21.0
21.5
22.0
22.5
23.0   ******
23.5
24.0
24.5
25.0
25.5   *********
26.0
```

2nd Example: X-diffraction pattern of diamond. Trigonal description with triple-hexagonal cell. Output A. Constants A, a, B, b and C for exponentical approximation of of the scattering factor are used.

COMPND	A	B	C	ALPHA	BETA	GAMMA
DIAMOND, DESCRIPTION SP. GR. R3BAR, 6 ATOMS/TRIPLE HEX. CELL, S.C. AT ORIG., MO K ALPH	2.5222/3		6.17793			

WL	SL	SH	NORM	ISCAT	IMAGE	KODLP	A GUIN	B GUIN
.71069		.2	1	0	1	0		

ISYSTM	IBRAVL	LAUE	ISYMCE	IHKO	IOKL	IHOL	IHHL	IHOO	IOKO	IOOL	NCOMPO	NA(1)	NA(2)	NA(3)	NA(4)	NA(5)	NA(6)	NA(7)	NA(8)
3	3	1	1	1	1	1	1	1	1	1	1	1							

ELEMT(1)	FOCCU(1)	AAA(1)	AA(1)	BBB(1)	BB(1)	CCC(1)	BTEMP(1)
C	2.	1.721	6.770	2.287	30.278	1.379	

X(1,1)	Y(1,1)	Z(1,1)
.0	.0	.375

```
INTENSITY CALCULATION FOR DIAMOND,DESCRIPTION SP.GR. R3BARM,6 ATOMS/TRIPLE HEX.CELL,S.C.AT ORIG.,MO K ALPH

DATA CALCULATED FOR A TRIGONAL STRUCTURE WITH
A=  2.52213,C=  6.17793,WL= 0.71069 ANGSTROM
 SIN-SQUARE-THETA-VALUES CALCULATED BETWEEN SL= 0.0    AND SH= 0.2000          KODLP= 0          AGUIN= 0.0        BGUIN= 0.0
RHOMBOHEDRAL BRAVAISLATTICE,HKL ONLY WITH -H+K+L=3N
SYMMETRY CENTER AT ORIGIN OF UNIT CELL
            ATOMS IN UNIT CELL: ELEMT(M)  NA(M)*NBRA*FOCCU(M)
                                C         1  * 3  *  2.00

COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF C       1.7210    6.7700    2.8870   30.2780    1.3790
BTEMP=   0.0     ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS    2.00000

C       0.0       0.0       0.37500   +(2/3 1/3 1/3,1/3 2/3 2/3)
```

H	K	L	THETA	2THETA	D-VALUE	SIN	SIN2*1000	H	K	L	INTENSITY	/F(HKL)/**2	A(HKL)	B(HKL)	PHA.ANG.	MULT	LPG
1	0	1	9.94	19.87	2.0593	0.1726	29.78	1	0	1	1000.0	164.0	-12.80	0.0	180.000	6.	64.25
0	0	3	9.94	19.87	2.0593	0.1726	29.78	0	0	3	333.3	164.0	12.80	0.0	0.0	2.	64.25
0	1	2	11.49	22.99	1.7834	0.1992	39.70	0	1	2	0.0	0.0	-0.00	0.0	180.000	6.	47.49
1	1	0	16.37	32.73	1.2611	0.2818	79.40	1	1	0	305.6	143.6	11.98	0.0	0.0	6.	22.41
1	0	4	16.37	32.73	1.2611	0.2818	79.40	1	0	4	305.6	143.6	-11.98	0.0	180.000	6.	22.41
1	1	3	19.29	38.59	1.0754	0.3304	109.18	1	1	3	84.8	57.1	7.56	0.0	0.0	6.	15.63
0	2	1	19.29	38.59	1.0754	0.3304	109.18	0	2	1	84.8	57.1	-7.56	0.0	180.000	6.	15.63
0	1	5	19.29	38.59	1.0754	0.3304	109.18	0	1	5	84.8	57.1	7.56	0.0	0.0	6.	15.63
1	1	-3	19.29	38.59	1.0754	0.3304	109.18	1	1	-3	84.8	57.1	7.56	0.0	0.0	6.	15.63
0	0	6	20.19	40.38	1.0297	0.3451	119.10	0	0	6	0.0	0.0	0.00	0.0	0.0	2.	14.14
2	0	2	20.19	40.38	1.0297	0.3451	119.10	2	0	2	0.0	0.0	-0.00	0.0	180.000	6.	14.14
0	2	4	23.49	46.97	0.8917	0.3985	158.80	0	2	4	86.3	90.3	-9.50	0.0	180.000	6.	10.06
2	0	5	25.74	51.48	0.8183	0.4363	188.58	2	0	5	32.1	41.4	6.43	0.0	0.0	6.	8.17
1	2	-1	25.74	51.48	0.8183	0.4363	188.58	1	2	-1	32.1	41.4	-6.43	0.0	180.000	6.	8.17
2	1	1	25.74	51.48	0.8183	0.4363	188.58	2	1	1	32.1	41.4	-6.43	0.0	180.000	6.	8.17
1	0	7	25.74	51.48	0.8183	0.4363	188.58	1	0	7	32.1	41.4	-6.43	0.0	180.000	6.	8.17
1	1	6	26.46	52.92	0.7976	0.4455	198.50	1	1	6	0.0	0.0	0.00	0.0	0.0	6.	7.67
2	1	-2	26.46	52.92	0.7976	0.4455	198.50	2	1	-2	0.0	0.0	-0.00	0.0	180.000	6.	7.67
1	2	2	26.46	52.92	0.7976	0.4455	198.50	1	2	2	0.0	0.0	-0.00	0.0	180.000	6.	7.67
1	1	-6	26.46	52.92	0.7976	0.4455	198.50	1	1	-6	0.0	0.0	0.00	0.0	0.0	6.	7.67

DIFFRACTION PATTERN FOR DIAMOND,DESCRIPTION SP.GR. R3DARH,6 ATOMS/TRIPLE HEX.CELL,S.C.AT ORIG.,MO K ALPH WL= 0.71069

```
 0.0
 0.5
 1.0
 1.5
 2.0
 2.5
 3.0
 3.5
 4.0
 4.5
 5.0
 5.5
 6.0
 6.5
 7.0
 7.5
 8.0
 8.5
 9.0
 9.5   ************************************************************************************************
10.0
10.5
11.0
11.5
12.0
12.5
13.0
13.5
14.0
14.5
15.0
15.5
16.0   ********************************************
16.5
17.0
17.5
18.0
18.5
19.0   ***************************
19.5
20.0
20.5
21.0
21.5
22.0
22.5
23.0   ******
23.5
24.0
24.5
25.0
25.5   *********
26.0
```

3rd Example: X-ray diffraction pattern of diamond. Triclinic cell without symmetry center at origin. Output B.

COMPND
DIAMOND, DESCRIPTION SP.GR. P1, 2 ATOMS/TRICL. CELL, NO S.C. AT ORIGIN, MO K ALPHA

A	B	C	ALPHA	BETA	GAMMA
2.52213	2.52215	2.52213	60.	60.	60.

WL	SL	SH	NORM	IS CAT	IMAGE	KODLP	A GUIN	B GUIN
.71069		.2	0	0	1	0		

ISYSTM	IBRAVL	LAUE	ISYMCE	IHKO	IOKL	IHOL	IHHL	IHOO	IOKO	IOOL	NCOMPO	NA(1)	NA(2)	NA(3)	NA(4)	NA(5)	NA(6)	NA(7)	NA(8)
7	1	1	0	1	1	1	1	1	1	1	1	2							

ELEMT(1)	FOCCU(1)	AAA (1)	AA (1)	BBB (1)	BB (1)	CCC (1)	BTEMP (1)
C		1.721	6.770	1.887	30.278	1.379	.

X (1,1)	Y (1,1)	Z (1,1)
.0	.0	.0

X (2,1)	Y (2,1)	Z (2,1)
.26	.26	.25

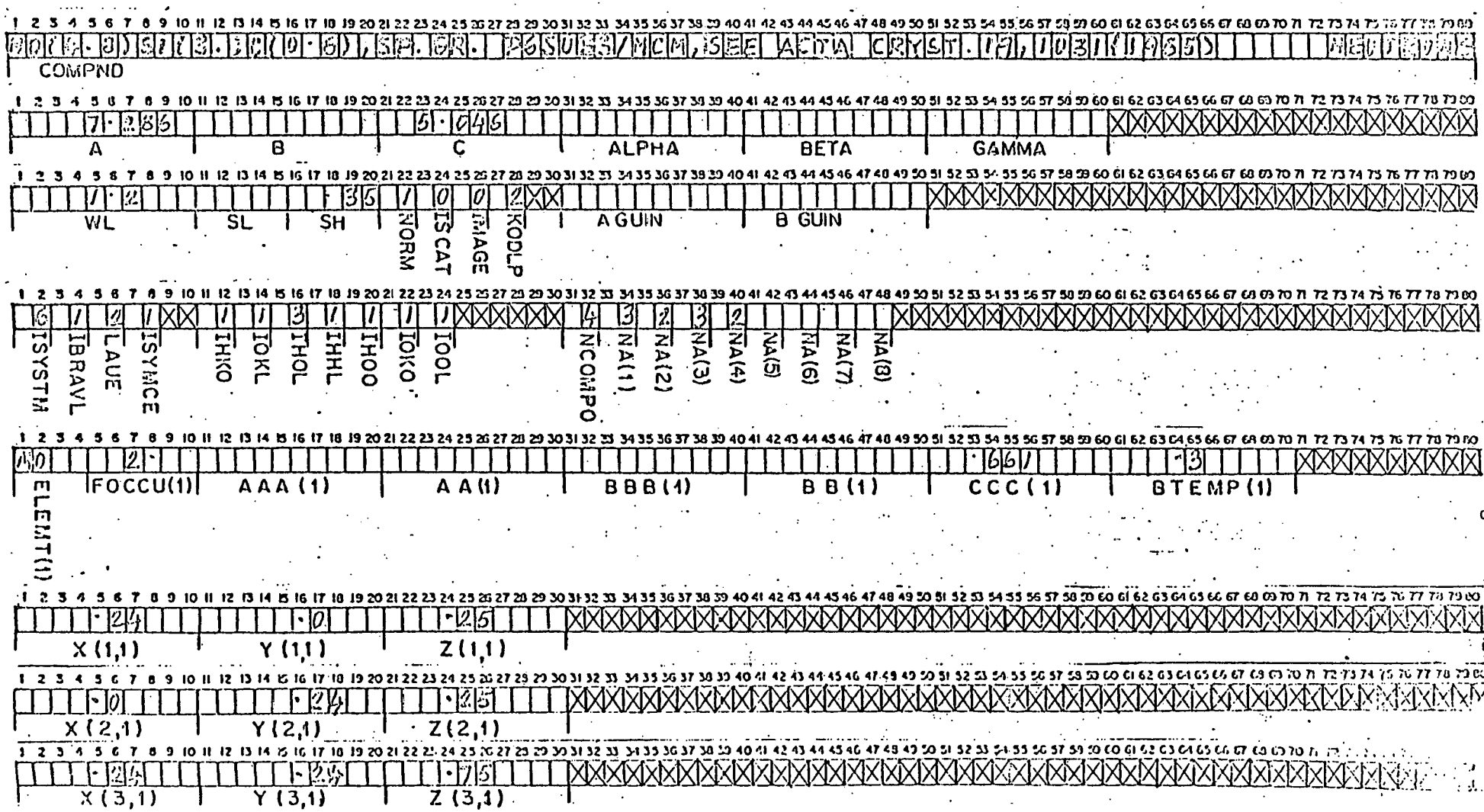
```
INTENSITY CALCULATION FOR DIAMOND,DESCRIPTION SP.GR. P1,2 ATOMS/TRICL. CELL,NO S.C. AT ORIGIN,  NO K ALPHA

DATA CALCULATED FOR A TRICLINIC STRUCTURE WITH
A=  2.52213,B=  2.52213,C=  2.52213,ALPHA= 60.00000,BETA= 60.00000,GAMMA= 60.00000,WL= 0.71069
 SIN-SQUARE-THETA-VALUES CALCULATED BETWEEN SL= 0.0    AND SH= 0.2000          KODLP= 0          AGUIN= 0.0        BGUIN= 0.0
PRIMITIVE BRAVAISLATTICE.ALL HKL VALUES ALLOWED
            ATOMS IN UNIT CELL: ELEMT(M)  NA(M)*NBRA*FOCCU(M)
                                C          2  *  1  *  1.00

COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF C        1.7210   6.7700    2.8870   30.2780    1.3790
BTEMP=   0.0      ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS     1.00000

C        0.0        0.0        0.0
C        0.25000    0.25000    0.25000
```

H	K	L	THETA	SIN2*1000	INT.SCALED	INTENSITY UNSCALED	/F(HKL)/**2	A(HKL)	B(HKL)	PHA.ANG.	MULT	LPG
1	1	1	9.94	29.78	1000.0	2341.1	18.2	3.02	-3.02	-45.000	2.	64.25
0	1	0	9.94	29.78	1000.0	2341.1	18.2	3.02	3.02	45.000	2.	64.25
0	0	1	9.94	29.78	1000.0	2341.1	18.2	3.02	3.02	45.000	2.	64.25
1	0	0	9.94	29.78	1000.0	2341.1	18.2	3.02	3.02	45.000	2.	64.25
1	0	1	11.49	39.70	0.0	0.0	0.0	0.0	0.00	90.000	2.	47.49
0	1	1	11.49	39.70	0.0	0.0	0.0	0.0	0.00	90.000	2.	47.49
1	1	0	11.49	39.70	0.0	0.0	0.0	0.0	0.00	90.000	2.	47.49
2	1	1	16.37	79.40	305.6	715.4	16.0	3.99	-0.00	-0.000	2.	22.41
1	2	1	16.37	79.40	305.6	715.4	16.0	3.99	-0.00	-0.000	2.	22.41
1	1	2	16.37	79.40	305.6	715.4	16.0	3.99	-0.00	-0.000	2.	22.41
1	0	-1	16.37	79.40	305.6	715.4	16.0	3.99	0.0	0.0	2.	22.41
0	1	-1	16.37	79.40	305.6	715.4	16.0	3.99	0.0	0.0	2.	22.41
1	-1	0	16.37	79.40	305.6	715.4	16.0	3.99	0.0	0.0	2.	22.41
2	2	1	19.29	109.18	84.8	198.5	6.3	1.78	1.78	45.000	2.	15.63
2	1	2	19.29	109.18	84.8	198.5	6.3	1.78	1.78	45.000	2.	15.63
1	2	2	19.29	109.18	84.8	198.5	6.3	1.78	1.78	45.000	2.	15.63
2	0	1	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
0	2	1	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
2	1	0	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
1	2	0	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
1	0	2	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
0	1	2	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
1	1	-1	19.29	109.18	84.8	198.5	6.3	1.78	1.78	45.000	2.	15.63
1	-1	1	19.29	109.18	84.8	198.5	6.3	1.78	1.78	45.000	2.	15.63
1	-1	-1	19.29	109.18	84.8	198.5	6.3	1.78	-1.78	-45.000	2.	15.63
2	2	2	20.19	119.10	0.0	0.0	0.0	0.0	0.00	90.000	2.	14.14
2	0	0	20.19	119.10	0.0	0.0	0.0	0.0	0.00	90.000	2.	14.14
0	2	0	20.19	119.10	0.0	0.0	0.0	0.0	0.00	90.000	2.	14.14
0	0	2	20.19	119.10	0.0	0.0	0.0	0.0	0.00	90.000	2.	14.14
0	2	2	23.48	158.80	86.3	202.0	10.0	3.17	-0.00	-0.000	2.	10.06
2	0	2	23.48	158.80	86.3	202.0	10.0	3.17	-0.00	-0.000	2.	10.06
2	2	0	23.48	158.80	86.3	202.0	10.0	3.17	-0.00	-0.000	2.	10.06
3	2	2	25.74	188.58	32.1	75.2	4.6	1.52	-1.52	-45.000	2.	8.17
2	3	2	25.74	188.58	32.1	75.2	4.6	1.52	-1.52	-45.000	2.	8.17
2	2	3	25.74	188.58	32.1	75.2	4.6	1.52	-1.52	-45.000	2.	8.17
3	1	1	25.74	188.58	32.1	75.2	4.6	1.52	1.52	45.000	2.	8.17
1	3	1	25.74	188.58	32.1	75.2	4.6	1.52	1.52	45.000	2.	8.17
1	1	3	25.74	188.58	32.1	75.2	4.6	1.52	1.52	45.000	2.	8.17
0	1	-2	25.74	188.58	32.1	75.2	4.6	1.52	-1.52	-45.000	2.	8.17
2	0	-1	25.74	188.58	32.1	75.2	4.6	1.52	1.52	45.000	2.	8.17
2	-1	0	25.74	188.58	32.1	75.2	4.6	1.52	1.52	45.000	2.	8.17
1	-2	0	25.74	188.58	32.1	75.2	4.6	1.52	-1.52	-45.000	2.	8.17
0	2	-1	25.74	188.58	32.1	75.2	4.6	1.52	1.52	45.000	2.	8.17
1	0	-2	25.74	188.58	32.1	75.2	4.6	1.52	-1.52	-45.000	2.	8.17
1	3	2	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
2	3	1	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
3	1	2	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
2	1	3	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
1	2	3	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
3	2	1	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
1	2	-1	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
2	-1	1	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
2	1	-1	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
1	-2	-1	26.46	198.50	0.0	0.0	0.0	0.0	-0.00	-90.000	2.	7.67
1	-1	2	26.46	198.50	0.0	0.0	0.0	0.0	0.00	90.000	2.	7.67
1	-1	-2	26.46	198.50	0.0	0.0	0.0	0.0	-0.00	-90.000	2.	7.67

DIFFRACTION PATTERN FOR DIAMOND,DESCRIPTION SP.GR. P1,2 ATOMS/TRICL. CELL,NO S.C. AT ORIGIN, NO K ALPHA WL= 0.71069

```
 0.0
 0.5
 1.0
 1.5
 2.0
 2.5
 3.0
 3.5
 4.0
 4.5
 5.0
 5.5
 6.0
 6.5
 7.0
 7.5
 8.0
 8.5
 9.0
 9.5   ****************************************************************************************************
10.0
10.5
11.0
11.5
12.0
12.5
13.0
13.5
14.0
14.5
15.0
15.5
16.0   ********************************************
16.5
17.0
17.5
18.0
18.5
19.0   ****************************
19.5
20.0
20.5
21.0
21.5
22.0
22.5
23.0   ******
23.5
24.0
24.5
25.0
25.5   *********
26.0
```

4th Example: Neutron diffraction pattern for $Mo_{4,8}Si_3C_{.6}$ Output A. For details on structure see Acta Cryst. 19, 1031 (1965).



19	1.8				66	1	3	
ELEMT(2)	FOCCU(2)	AAA(2)	AA(2)	BBB(2)	BB(2)	CCC(2)	BTEMP(2)	

3.5333	66666	0
X(1,2)	Y(1,2)	Z(1,2)
3.5333	66666	5
X(2,2)	Y(2,2)	Z(2,2)

91	2.				42		3	
ELEMT(3)	FOCCU(3)	AAA(3)	AA(3)	BBB(3)	BB(3)	CCC(3)	BTEMP(3)	

.6	.0	.25
X(1,3)	Y(1,3)	Z(1,3)
.0	.6	.25
X(2,3)	Y(2,3)	Z(2,3)
.6	.6	.75
X(3,3)	Y(3,3)	Z(3,3)

4	.6				661		3	
ELEMT(4)	FOCCU(4)	AAA(4)	AA(4)	BBB(4)	BB(4)	CCC(4)	BTEMP(4)	

.0	.0	.0
X(1,4)	Y(1,4)	Z(1,4)
.0	.0	.5
X(2,4)	Y(2,4)	Z(2,4)

```
INTENSITY CALCULATION FOR MO(4.8)SI(3.)C(0.6),SP.GR. P6SUB3/MCM SEE ACTA CRYST.19,1031(1965)      NEUTRONS

DATA CALCULATED FOR A HEXAGONAL STRUCTURE WITH
A=  7.28600,C=  5.04600,WL= 1.20000 ANGSTROM
 SIN-SQUARE-THETA-VALUES CALCULATED BETWEEN SL= 0.0    AND SH= 0.300          KODLP= 2          AGUIN= 0.0        BGUIN= 0.0
DATA CALCULATED FOR HIGH LAUE-SYMMETRY
PRIMITIVE BRAVAISLATTICE.ALL HKL VALUES ALLOWED
HKL ONLY WITH L=2N
SYMMETRY CENTER AT ORIGIN OF UNIT CELL
          ATOMS IN UNIT CELL: ELEM(M)  NA(M)*NORA*FOCCU(M)
                              MO        3  * 1  *  2.00
                              MO        2  * 1  *  1.00
                              SI        3  * 1  *  2.00
                              C         2  * 1  *  0.60

COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF MO      0.0       0.0       0.0       0.0       0.6610
BTEMP=   0.30000 ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS    2.00000

MO      0.24000   0.0       0.25000
MO      0.0       0.24000   0.25000
MO      0.24000   0.24000   0.75000

COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF MO      0.0       0.0       0.0       0.0       0.6610
BTEMP=   0.30000 ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS    1.80000

MO      0.33333   0.66667   0.0
MO      0.33333   0.66667   0.50000

COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF SI      0.0       0.0       0.0       0.0       0.4200
BTEMP=   0.30000 ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS    2.00000

SI      0.60000   0.0       0.25000
SI      0.0       0.60000   0.25000
SI      0.60000   0.60000   0.75000

COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF C       0.0       0.0       0.0       0.0       0.6610
BTEMP=   0.30000 ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS    0.60000

C       0.0       0.0       0.0
C       0.0       0.0       0.50000
```

H	K	L	THETA	2THETA	D-VALUE	SIN	SIN2*1000	H	K	L	INTENSITY	/F(HKL)/**2	A(HKL)	B(HKL)	PHA.ANG.	MULT	LPG
1	0	0	5.46	10.91	6.3099	0.0951	9.04	1	0	0	46.1	0.3	0.57	0.0	0.0	6.	111.10
1	1	0	9.48	18.96	3.6430	0.1647	27.13	1	1	0	40.4	0.9	0.92	0.0	0.0	6.	37.38
2	0	0	10.96	21.93	3.1549	0.1902	36.17	2	0	0	4.0	0.1	-0.34	0.0	180.000	6.	28.16
1	1	1	11.72	23.44	2.9537	0.2031	41.26	1	1	1	29.2	0.5	-0.68	0.0	180.000	12.	24.75
0	0	2	13.76	27.51	2.5230	0.2370	56.55	0	0	2	82.7	10.7	-3.27	0.0	180.000	2.	18.20
2	1	0	14.57	29.14	2.3849	0.2516	63.29	2	1	0	167.0	4.0	-2.01	0.0	180.000	12.	16.32
1	0	2	14.84	29.68	2.3427	0.2561	65.60	1	0	2	72.7	1.8	-1.35	0.0	180.000	12.	15.77
2	1	1	16.16	32.31	2.1562	0.2783	77.43	2	1	1	1000.0	14.6	-3.83	0.0	180.000	24.	13.45
3	0	0	16.57	33.15	2.1033	0.2853	81.38	3	0	0	452.1	27.8	5.27	0.0	0.0	6.	12.82
1	1	2	16.81	33.63	2.0741	0.2893	83.68	1	1	2	899.3	28.3	5.32	0.0	0.0	12.	12.48
2	0	2	17.73	35.46	1.9704	0.3045	92.72	2	0	2	5.7	0.2	-0.45	0.0	180.000	12.	11.32
2	2	0	19.23	38.46	1.8215	0.3294	108.50	2	2	0	33.0	2.7	1.63	0.0	0.0	6.	9.76
3	1	0	20.05	40.10	1.7500	0.3428	117.55	3	1	0	3.2	0.1	-0.37	0.0	180.000	12.	9.06
2	1	2	20.25	40.51	1.7331	0.3462	119.85	2	1	2	66.1	1.5	1.21	0.0	0.0	24.	8.89
2	2	1	20.50	41.00	1.7133	0.3502	122.64	2	2	1	65.4	3.0	-1.72	0.0	180.000	12.	8.71
3	1	1	21.28	42.55	1.6534	0.3629	131.68	3	1	1	80.9	2.0	1.40	0.0	0.0	24.	8.15
3	0	2	21.80	43.60	1.6155	0.3714	137.93	3	0	2	18.3	0.9	0.96	0.0	0.0	12.	7.81
4	0	0	22.36	44.71	1.5775	0.3804	144.67	4	0	0	78.7	8.3	2.88	0.0	0.0	6.	7.47
1	1	3	23.14	46.27	1.5271	0.3929	154.37	1	1	3	7.9	0.4	0.66	0.0	0.0	12.	7.04
2	2	2	23.97	47.94	1.4768	0.4063	165.06	2	2	2	343.9	20.4	4.52	0.0	0.0	12.	6.63
3	2	0	24.49	48.97	1.4476	0.4145	171.80	3	2	0	0.5	0.0	-0.18	0.0	180.000	12.	6.40
3	1	2	24.66	49.32	1.4380	0.4173	174.10	3	1	2	5.1	0.2	-0.40	0.0	180.000	24.	6.32
3	2	1	25.54	51.09	1.3915	0.4312	185.94	3	2	1	160.2	5.3	2.30	0.0	0.0	24.	5.96
4	1	0	25.83	51.67	1.3769	0.4358	189.88	4	1	0	269.1	10.1	4.25	0.0	0.0	12.	5.85
2	1	3	25.88	51.76	1.3745	0.4365	190.54	2	1	3	413.9	14.0	3.74	0.0	0.0	24.	5.83
4	0	2	26.65	53.31	1.3375	0.4486	201.23	4	0	2	183.7	13.0	-3.61	0.0	180.000	12.	5.56
4	1	1	26.85	53.70	1.3284	0.4517	204.02	4	1	1	1.0	0.1	0.26	0.0	0.0	24.	5.49
5	0	0	28.39	56.78	1.2620	0.4754	226.05	5	0	0	105.6	16.5	4.07	0.0	0.0	6.	5.03
0	0	4	28.40	56.80	1.2615	0.4756	226.22	0	0	4	180.7	84.9	9.21	0.0	0.0	2.	5.03
3	2	2	28.55	57.09	1.2556	0.4779	228.35	3	2	2	8.4	0.3	-0.58	0.0	180.000	24.	4.99
1	0	4	29.01	58.03	1.2370	0.4850	235.26	1	0	4	3.7	0.3	0.54	0.0	0.0	12.	4.86
2	2	3	29.05	58.10	1.2357	0.4855	235.75	2	2	3	34.8	2.8	1.68	0.0	0.0	12.	4.85
3	3	0	29.61	59.22	1.2143	0.4941	244.13	3	3	0	9.0	1.5	1.22	0.0	0.0	6.	4.71
3	1	3	29.65	59.31	1.2127	0.4948	244.79	3	1	3	44.5	1.9	-1.37	0.0	180.000	24.	4.70
4	1	2	29.76	59.53	1.2086	0.4964	246.44	4	1	2	79.0	3.3	1.82	0.0	0.0	24.	4.67
4	2	0	30.21	60.42	1.1925	0.5032	253.17	4	2	0	79.4	6.8	-2.62	0.0	180.000	12.	4.57
1	1	4	30.22	60.44	1.1921	0.5033	253.34	1	1	4	9.0	0.8	0.88	0.0	0.0	12.	4.57
3	3	1	30.54	61.09	1.1806	0.5082	258.27	3	3	1	179.9	15.7	3.97	0.0	0.0	12.	4.50
2	0	4	30.81	61.63	1.1713	0.5122	262.39	2	0	4	1.2	0.1	-0.32	0.0	180.000	12.	4.44
4	2	1	31.13	62.27	1.1605	0.5170	267.31	4	2	1	25.7	1.2	-1.08	0.0	180.000	24.	4.37
5	1	0	31.97	63.93	1.1333	0.5294	280.30	5	1	0	26.0	2.4	-1.56	0.0	180.000	12.	4.21
5	0	2	32.11	64.23	1.1287	0.5316	282.60	5	0	2	241.2	22.7	-4.77	0.0	180.000	12.	4.18
2	1	4	32.55	65.10	1.1151	0.5381	289.51	2	1	4	76.3	3.7	-1.91	0.0	180.000	24.	4.10
5	1	1	32.86	65.72	1.1057	0.5426	294.44	5	1	1	79.4	3.9	-1.97	0.0	180.000	24.	4.04
3	2	3	33.15	66.30	1.0972	0.5469	299.04	3	2	3	102.4	5.0	-2.25	0.0	180.000	24.	3.99
3	3	2	33.25	66.51	1.0942	0.5483	300.69	3	3	2	228.1	22.6	4.75	0.0	0.0	12.	3.98
3	0	4	33.68	67.37	1.0810	0.5546	307.60	3	0	4	250.8	25.3	5.03	0.0	0.0	12.	3.91
4	2	2	33.82	67.63	1.0781	0.5565	309.73	4	2	2	66.9	3.4	1.84	0.0	0.0	24.	3.89
4	1	3	34.27	68.55	1.0655	0.5631	317.13	4	1	3	1.2	0.1	-0.25	0.0	180.000	24.	3.82
6	0	0	34.79	69.58	1.0516	0.5705	325.51	6	0	0	9.6	2.0	1.42	0.0	0.0	6.	3.74
4	3	0	35.34	70.68	1.0373	0.5784	334.55	4	3	0	0.1	0.0	-0.08	0.0	180.000	12.	3.66
2	2	4	35.35	70.70	1.0371	0.5786	334.72	2	2	4	22.6	2.4	1.56	0.0	0.0	12.	3.66
5	1	2	35.48	70.96	1.0338	0.5804	336.85	5	1	2	11.9	0.6	0.80	0.0	0.0	24.	3.65
3	1	4	35.90	71.79	1.0233	0.5863	343.76	3	1	4	2.3	0.1	-0.35	0.0	180.000	24.	3.59
4	3	1	36.19	72.39	1.0161	0.5905	348.69	4	3	1	36.8	2.0	1.43	0.0	0.0	24.	3.55

F) Appendix.

Copy of tables from a paper by F. H. Moore in Acta Cryst 16, 1169 (1963) which contain the constants for the exponential structure factor approximation.

$$f\left(\frac{\sin\theta}{\lambda}\right) = Ae^{-a\left(\frac{\sin^2\theta}{\lambda^2}\right)} + Be^{-b\left(\frac{\sin^2\theta}{\lambda^2}\right)} + C$$

Table 1. *Analytic constants for atomic scattering factors derived from self-consistent or variational wave functions*

Element	CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
	A	*a*	*B*	*b*	*C*	*c*	*A*	*a*	*B*	*b*	*C*	*c*
H	0.4629	9.077	0.5148	33.154	0.0207	0.167	0.3356	6.381	0.6543	27.870	0.0055	0.300
H^{-1}	1.003	17.616	0.9367	183.64	0.0477	0.959	0.9195	14.275	1.039	151.50	0.0142	0.508
He	1.253	4.808	0.6041	19.319	0.1314	0.071	0.9138	2.930	1.037	13.275	0.0388	0.314
He^{-1}	1.678	7.866	1.073	1147.0	0.2489	0.687	1.745	5.873	1.165	829.12	0.0880	1.468
Li	1.575	3.404	1.064	114.93	0.3564	0.135	1.689	2.601	1.121	101.23	0.1755	0.600
Li^{+1}	1.416	2.466	0.3651	8.636	0.2190	0.011	1.132	1.583	0.7798	5.968	0.0850	0.074
Li^{-1}	1.527	4.633	1.934	309.68	0.5235	1.006	1.742	2.824	2.023	265.05	0.1973	1.060
Be	1.351	2.315	2.032	55.970	0.6032	0.252	1.649	1.501	2.086	53.191	0.2443	0.257
Be^{+1}	1.414	2.205	1.037	44.837	0.5446	0.127	1.637	1.544	1.073	40.979	0.2595	0.275
Be^{+2}	1.469	1.583	0.2155	5.193	0.3159	0.014	1.297	1.046	0.5663	3.626	0.1354	0.029
B	1.093	4.493	2.721	37.231	1.169	0.294	1.575	1.130	3.009	32.460	0.3747	0.400
B^{+1}	1.028	2.521	1.979	28.552	0.9378	0.125	1.566	0.9904	2.098	26.479	0.3218	0.188
B^{+2}	1.184	1.546	0.9906	24.522	0.8232	0.070	1.582	1.041	1.077	22.105	0.3327	0.167
B^{+3}	1.472	1.357	0.0103	11.025	0.5174	0.021	1.404	0.7550	0.4113	2.529	0.1844	0.012
C	1.620	6.785	2.988	28.126	1.380	0.211	1.407	1.119	3.907	21.701	0.6328	0.483
C(valence)	1.721	6.770	2.857	30.278	1.379	0.212	1.469	1.253	3.817	22.765	0.6543	0.531
C^{+2}	0.8819	3.095	1.881	16.337	1.236	0.047	1.319	0.6231	2.159	14.460	0.3119	0.154
C^{+3}	1.003	2.113	0.9051	16.139	1.091	0.029	1.515	0.7724	1.065	13.837	0.4134	0.130
C^{+4}	1.590	0.8103	0.0209	6.088	0.3657	0.022	1.335	0.4187	0.5712	1.465	0.0935	0.024
N	2.708	7.081	2.810	23.810	1.474	0.105	1.383	1.581	4.612	16.297	0.9449	0.470
N^{+3}	1.102	3.734	1.519	13.090	1.379	0.016	1.325	0.6504	2.073	10.645	0.5909	0.145
N^{+4}	0.9459	2.130	0.8156	11.595	1.237	0.014	1.417	0.6427	1.043	9.691	0.5339	0.098
N^{-1}	3.594	9.051	2.855	40.533	1.534	0.292	1.886	3.551	4.817	24.559	1.205	0.651
O	3.811	6.363	2.633	21.191	1.550	0.055	1.841	2.342	4.546	13.822	1.160	0.418
O^{+1}	3.115	5.368	2.390	15.357	1.492	0.023	1.682	2.558	4.065	11.431	1.234	0.179
O^{+2}	2.499	4.673	2.042	12.366	1.459	0.012	1.344	2.009	3.453	9.551	1.190	0.121
O^{+3}	1.921	4.024	1.648	10.358	1.431	0.010	1.091	1.538	2.760	8.187	1.142	0.082
O^{-1}	4.551	7.554	2.818	32.818	1.614	0.158	2.912	4.249	4.006	21.356	1.331	0.467
F	4.824	5.530	2.477	19.362	1.636	0.048	3.340	3.553	4.254	13.813	1.377	0.218
F^{-1}	4.735	5.461	3.612	19.260	1.609	0.039	2.793	2.623	5.917	13.665	1.238	0.387
Ne	3.519	4.538	2.770	15.057	1.706	0.021	3.335	2.467	5.327	10.248	1.302	0.261
Na	7.504	5.179	1.275	107.08	2.203	0.213	7.303	3.753	1.987	39.203	1.553	0.803
Na^{+}	6.298	3.751	1.938	11.842	1.754	0.008	3.956	2.225	4.677	7.640	1.345	0.159
Mg	7.459	3.979	2.272	73.153	2.254	0.110	7.664	3.122	2.657	54.177	1.613	0.546
Mg^{+2}	6.807	3.436	1.183	9.452	2.007	0.048	4.360	1.970	4.240	6.014	1.392	0.069
Al	7.373	3.173	3.246	60.771	2.334	0.150	7.745	2.434	3.569	50.689	1.615	0.437
Al^{+1}	7.458	2.549	2.409	45.721	2.126	0.072	7.610	2.391	2.623	36.554	1.782	0.199
Al^{+2}	7.483	2.559	1.351	32.039	2.134	0.038	7.320	2.135	1.011	22.314	1.627	0.307
Al^{+3}	6.049	2.833	2.111	6.088	1.679	0.023	5.130	1.759	3.613	5.037	1.313	0.033

Table 1 (cont.)

Element		CuK, radiation						MoK, radiation					
		A	a	B	b	C	c	A	a	B	b	C	c
Si		7.180	2.619	4.299	45.092	2.494	0.150	7.725	2.033	4.576	41.411	1.641	0.287
	Si^{+3}	7.559	2.341	1.403	22.953	2.044	0.029	7.630	2.134	1.587	19.970	1.771	0.095
	Si^{+4}	7.034	2.180	0.9823	5.989	1.934	0.012	5.054	1.439	3.534	3.938	1.412	0.017
P		6.792	2.344	5.297	36.132	2.882	0.150	7.705	1.681	5.588	33.628	1.652	0.204
S		7.545	1.328	6.821	25.077	1.627	0.036	7.700	1.308	6.805	26.003	1.489	0.049
	S^{-1}	8.161	1.135	7.940	27.268	0.8936	0.036	7.688	1.283	7.860	27.675	1.452	0.058
	S^{-2}	13.116	0.6088	8.944	37.448	-4.048	0.069	7.893	1.251	8.740	38.886	1.397	0.159
Cl		7.239	1.138	7.937	22.203	1.819	0.044	7.717	1.070	7.916	22.367	1.367	0.078
	Cl^{-}	7.722	1.002	9.023	23.413	1.246	0.036	7.681	1.069	8.936	23.809	1.385	0.096
Ar		5.394	3.207	7.462	22.232	5.124	0.109	7.479	1.040	8.686	19.039	1.761	0.220
K		9.494	7.931	3.012	64.361	6.461	0.575	7.304	0.9700	9.257	16.525	2.027	0.677
	K^{+1}	3.213	3.254	7.321	16.861	5.457	0.057	7.406	0.8352	8.932	14.310	1.609	0.156
Ca		10.256	7.667	3.060	90.954	6.639	0.358	7.111	1.303	9.073	16.811	3.128	1.170
	Ca^{+1}	9.635	6.878	2.836	45.260	6.490	0.336	7.039	0.9194	9.304	13.407	2.328	0.598
	Ca^{+2}	5.101	2.820	7.432	13.167	5.460	0.035	7.317	0.7105	9.070	11.361	1.576	0.105
Sc		10.966	7.405	3.169	54.359	6.791	0.335	7.055	1.006	10.614	14.092	2.812	0.834
	Sc^{+1}	9.183	5.839	4.287	23.602	6.436	0.140	7.069	0.7983	10.477	12.008	2.256	0.406
	Sc^{+2}	7.056	4.436	5.756	14.789	6.179	0.047	7.211	0.6655	9.955	10.421	1.759	0.191
	Sc^{+3}	5.540	3.235	6.537	11.243	5.820	0.022	7.404	0.5732	9.255	9.187	1.307	0.103
Ti		11.690	6.680	3.408	70.858	6.855	0.257	7.151	1.308	10.512	14.446	3.654	1.129
	Ti^{+1}	10.252	5.769	4.087	23.309	6.625	0.110	6.793	0.8491	11.220	11.024	2.779	0.434
	Ti^{+2}	8.812	4.652	4.782	15.868	6.396	0.043	6.851	0.6938	10.738	9.611	2.295	0.251
	Ti^{+3}	7.186	3.917	5.659	11.822	6.150	0.020	6.932	0.6018	10.071	8.541	1.835	0.148
V		12.536	6.298	3.443	65.724	6.976	0.231	7.468	1.532	10.711	13.937	4.173	1.090
	V^{+1}	11.215	5.518	4.027	22.517	6.737	0.088	6.596	0.9651	11.204	10.295	3.390	0.443
	V^{+2}	10.173	4.834	4.270	16.209	6.549	0.034	6.527	0.7751	11.440	8.927	2.918	0.282
	V^{+3}	8.334	3.945	5.402	11.708	6.259	0.023	6.617	0.6470	10.845	7.949	2.475	0.181
Cr		13.530	5.993	3.336	43.358	7.087	0.189	7.343	1.471	11.866	11.864	4.343	0.778
	Cr^{+1}	12.165	5.227	3.991	21.235	6.826	0.071	6.581	1.085	12.338	9.591	3.878	0.434
	Cr^{+2}	11.234	4.694	4.119	15.858	6.638	0.035	6.335	0.9116	11.972	8.369	3.573	0.290
	Cr^{+3}	9.932	4.109	4.623	12.067	6.443	0.013	6.245	0.7527	11.495	7.449	3.190	0.200
Mn		14.310	5.599	3.413	58.160	7.228	0.194	9.191	2.055	10.289	13.782	4.943	0.956
	Mn^{+1}	13.074	4.931	3.955	20.498	6.926	0.062	6.901	1.284	12.529	9.215	4.372	0.427
	Mn^{+2}	12.007	4.411	4.280	14.550	6.707	0.020	6.422	1.289	11.959	8.167	4.515	0.247
	Mn^{+3}	10.997	3.996	4.445	11.713	6.554	0.009	6.129	0.8819	12.021	7.035	3.779	0.201
	Mn^{+4}	9.936	3.661	4.627	9.486	6.435	0.013	5.773	0.8352	11.383	6.375	3.807	0.110
Fe		15.133	5.270	3.444	54.196	7.379	0.179	10.605	2.305	9.642	14.368	5.249	0.885
	Fe^{+1}	14.018	4.693	3.914	19.763	7.055	0.053	7.493	1.467	12.584	8.904	4.739	0.412
	Fe^{+2}	13.224	4.293	3.925	14.841	6.845	0.017	6.712	1.214	12.675	7.588	4.439	0.279
	Fe^{+3}	12.364	3.952	3.950	11.615	6.685	0.014	6.240	1.197	12.101	6.791	4.601	0.166
	Fe^{+4}	11.647	3.386	4.317	9.009	6.436	0.008	5.987	0.8712	11.978	6.023	3.592	0.137
Co		15.524	4.979	3.414	51.757	7.551	0.168	12.022	2.453	9.056	14.861	5.463	0.801
	Co^{+1}	14.832	4.422	3.933	18.624	7.140	0.043	8.335	1.626	12.477	8.609	5.017	0.371
	Co^{+2}	14.052	4.009	4.045	14.069	6.830	0.019	7.326	1.360	12.782	7.310	4.805	0.267
	Co^{+3}	13.008	3.651	4.209	11.542	6.703	0.010	6.637	1.139	12.695	6.341	4.602	0.171

Table 1 (*cont.*)

Element		CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
		A	a	B	b	C	c	A	a	B	b	C	c
Ni		16.859	4.749	3.365	49.734	7.734	0.160	13.358	2.529	8.580	15.113	5.643	0.739
	Ni^{+1}	15.762	4.191	3.935	17.856	7.294	0.031	9.383	1.758	12.224	8.501	5.242	0.332
	Ni^{+2}	14.982	3.813	4.008	13.447	7.005	0.016	8.133	1.492	12.711	7.091	5.058	0.239
	Ni^{+3}	14.274	3.583	3.851	11.011	6.877	0.009	7.299	1.303	12.739	6.189	4.900	0.173
Cu		17.815	4.537	3.239	33.810	7.997	0.127	12.957	2.264	10.024	11.554	5.654	0.319
	Cu^{+1}	16.595	3.896	4.051	17.041	7.345	0.034	11.819	2.175	10.367	9.250	5.703	0.254
	Cu^{+2}	15.988	3.665	3.851	13.139	7.151	0.011	9.155	1.609	12.481	6.927	5.276	0.221
	Cu^{+3}	15.043	3.337	4.054	10.299	6.902	0.009	8.158	1.418	12.657	5.991	5.127	0.157
Zn		18.543	4.299	3.260	46.229	8.156	0.135	15.864	2.520	7.655	15.264	5.915	0.610
	Zn^{+2}	16.892	3.421	3.931	12.782	7.205	0.013	11.821	2.001	10.395	7.501	5.720	0.160
Ga		18.653	3.890	4.003	47.443	8.291	0.147	18.212	2.628	6.376	23.516	6.113	0.598
	Ga^{+1}	18.509	3.674	3.491	31.007	7.978	0.067	16.341	2.331	7.501	13.645	5.932	0.435
	Ga^{+3}	17.277	3.114	3.499	10.420	7.224	0.009	10.844	1.639	11.539	5.901	5.507	0.133
Ge		18.762	3.483	4.884	43.735	8.311	0.122	18.997	2.495	6.591	27.676	6.194	0.514
	Ge^{+2}	18.678	3.243	3.435	24.385	7.876	0.038	17.211	2.220	6.645	12.779	5.591	0.346
	Ge^{+4}	16.955	2.638	4.129	7.880	6.917	0.009	12.034	1.708	10.222	5.384	5.723	0.066
As		18.756	3.106	5.892	37.993	8.300	0.101	19.320	2.301	7.287	27.846	6.222	0.413
	As^{+1}	18.575	3.244	5.098	36.062	8.300	0.092	18.619	2.410	6.786	23.589	6.432	0.380
	As^{+2}	18.524	3.158	4.336	28.190	8.128	0.047	18.123	2.327	6.393	17.823	6.353	0.321
	As^{+3}	18.425	3.038	3.683	20.998	7.836	0.023	17.283	2.204	6.372	12.589	6.241	0.250
	As^{+5}	17.779	2.502	3.193	7.192	7.028	0.006	12.012	1.566	10.270	4.628	5.702	0.043
Se		18.662	2.849	6.835	33.858	8.465	0.095	19.531	2.113	8.105	26.700	6.218	0.330
	Se^{+6}	17.364	2.173	3.739	5.708	6.837	0.009	12.165	1.454	10.136	4.069	5.690	0.031
Br		18.394	2.644	7.207	29.824	8.756	0.086	19.594	1.923	9.055	24.568	6.225	0.253
	Br^{+7}	19.069	2.222	1.685	6.459	7.249	0.009	12.523	1.374	9.755	3.642	5.703	0.022
	Br^{-1}	18.251	2.845	8.393	35.668	9.287	0.157	19.795	1.959	9.743	29.767	6.271	0.322
Kr		18.032	2.507	8.753	26.563	9.183	0.081	19.637	1.755	10.053	22.454	6.155	0.207
	Kr^{+8}	14.567	0.5346	13.258	3.007	0.166	0.007	12.435	1.251	9.923	3.224	5.640	0.011
	Rb^{+1}	17.861	2.211	9.099	20.791	9.023	0.041	19.493	1.606	10.221	18.450	6.221	0.115
	Sr^{+4}	17.348	1.740	9.630	13.539	9.015	0.015	19.313	1.251	10.701	12.471	5.957	0.030
	Zr^{+4}	17.301	3.817	8.790	28.572	14.824	0.209	19.941	1.193	14.207	16.386	6.455	0.384
Ag		20.137	4.645	9.296	24.870	17.493	0.128	18.850	1.088	19.051	12.979	8.652	0.442
	Ag^{+1}	19.105	3.839	10.204	16.346	16.662	0.045	18.551	0.9245	19.534	10.306	7.698	0.245
Cd		36.594	3.647	9.202	42.974	28.065	0.244	38.655	1.579	17.935	16.338	16.500	0.459
	Cd^{+}	35.524	3.050	13.033	21.945	29.372	0.079	39.445	1.339	21.104	13.806	17.049	0.257
In		36.733	3.453	11.590	29.761	31.546	0.133	39.928	1.442	20.536	15.477	18.855	0.408
	In^{+2}	35.913	3.109	11.917	20.264	30.171	0.079	38.680	1.310	21.310	12.107	17.713	0.248
	Tl^{+1}	36.608	3.436	11.577	25.631	31.706	0.129	39.463	1.261	22.529	12.894	17.391	0.335
	Tl^{+3}	34.663	2.491	15.112	14.748	28.202	0.027	38.676	1.149	22.695	10.657	16.420	0.151
	Pb^{+3}	35.265	3.028	11.531	17.737	30.805	0.067	39.019	1.144	22.895	10.551	16.822	0.213
	U^{+6}	39.590	2.222	14.811	17.162	31.191	0.008	42.286	1.348	20.421	12.533	23.051	0.252

Table 2. *Analytic constants for atomic scattering factors derived from Thomas–Fermi–Dirac statistics*

Element	CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
	A	a	B	b	C	c	A	a	B	b	C	c
Ca	9.625	4.447	4.752	36.621	5.609	0.164	9.092	1.954	7.399	20.736	3.291	0.719
Ca^{+1}	8.707	3.082	5.565	20.204	4.733	0.033						
Ca^{+2}	8.932	1.339	7.056	11.919	2.013	0.020						
Sc	10.115	4.429	4.899	36.471	5.371	0.151	9.351	1.928	7.704	20.626	3.504	0.703
Sc^{+1}	9.211	3.056	5.759	20.372	5.027	0.030						
Sc^{+2}	9.605	1.324	7.348	12.110	2.049	0.020						
Sc^{+3}	67.014	0.0782	8.542	8.107	−57.555	0.014						
Ti	10.586	4.382	5.072	36.264	6.323	0.161	10.063	1.920	7.566	20.353	3.729	0.693
Ti^{+1}	9.691	3.144	5.975	20.747	5.440	0.030						
Ti^{+2}	9.646	1.539	7.397	12.539	2.963	0.025						
Ti^{+3}	35.927	0.1055	8.801	8.340	−45.728	0.013						
V	11.075	4.347	5.230	36.060	6.674	0.159	10.521	1.894	8.281	20.017	3.941	0.693
V^{+1}	10.200	3.137	6.056	20.948	5.754	0.033						
V^{+2}	9.974	1.624	7.588	12.749	3.442	0.026						
V^{+3}	71.040	0.0373	9.195	8.460	−60.235	0.011						
Cr	11.550	4.324	5.381	35.543	7.046	0.162	11.009	1.877	8.563	19.839	4.159	0.683
Cr^{+1}	10.653	3.205	6.172	21.205	6.191	0.032						
Cr^{+2}	10.303	1.754	7.681	13.099	4.021	0.028						
Cr^{+3}	17.330	0.4676	9.166	8.823	−5.494	0.015						
Mn	12.043	4.333	5.492	36.078	7.443	0.158	11.485	1.860	8.851	19.616	4.303	0.682
Mn^{+1}	11.153	3.183	6.363	21.361	6.493	0.031						
Mn^{+2}	10.785	1.800	7.859	13.316	4.352	0.022						
Mn^{+3}	16.119	0.5639	9.336	9.066	−3.452	0.014						
Mn^{+4}	181.856	0.0279	10.089	6.723	−170.942	0.015						
Fe	12.517	4.293	5.651	35.880	7.806	0.157	11.986	1.851	9.103	19.513	4.614	0.676
Fe^{+1}	11.639	3.196	6.510	21.504	6.857	0.023						
Fe^{+2}	11.143	1.904	7.959	13.595	4.893	0.023						
Fe^{+3}	19.639	0.4759	9.728	9.163	−6.363	0.012						
Fe^{+4}	151.727	0.0358	10.451	6.846	−140.176	0.013						
Co	12.992	4.275	5.791	35.728	8.188	0.161	12.448	1.831	9.404	19.258	4.841	0.671
Co^{+1}	12.147	3.243	6.603	21.861	7.259	0.027						
Co^{+2}	11.684	1.901	8.196	13.733	5.125	0.019						
Co^{+3}	13.149	0.9294	9.523	9.583	1.333	0.018						
Ni	13.467	4.234	5.952	35.577	8.555	0.155	12.954	1.820	9.682	19.101	5.073	0.657
Ni^{+1}	12.608	3.253	6.760	21.937	7.638	0.025						
Ni^{+2}	12.250	1.910	8.382	13.926	5.374	0.020						
Ni^{+3}	17.779	0.6352	10.132	9.523	−2.910	0.014						
Cu	13.943	4.234	6.069	35.505	8.958	0.159	13.414	1.806	9.949	18.549	5.310	0.661
Cu^{+1}	13.095	3.235	6.934	22.049	7.977	0.018						
Cu^{+2}	12.543	1.973	8.529	14.097	5.830	0.019						
Cu^{+3}	15.243	0.8504	10.213	9.730	0.5434	0.015						
Zn	14.425	4.199	6.218	35.382	9.327	0.161	13.906	1.793	10.210	18.823	5.547	0.650
Zn^{+2}	13.539	1.697	9.250	13.509	5.297	0.024						
Ga	14.903	4.202	6.319	35.453	9.751	0.162	14.388	1.783	10.473	18.639	5.726	0.633
Ga^{+1}	14.047	3.263	7.169	22.422	8.750	0.017						
Ga^{+3}	13.403	1.136	10.315	10.239	3.283	0.009						

Table 2 (*cont.*)

Element	CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
	A	*a*	*B*	*b*	*C*	*c*	*A*	*a*	*B*	*b*	*C*	*c*
Ge	15.334	4.171	6.460	35.371	10.120	0.160	14.868	1.758	10.746	18.509	6.021	0.655
Ge^{+2}	13.944	2.165	8.240	14.777	7.224	0.022						
Ge^{+4}	61.544	0.1385	12.182	7.654	-45.725	0.012						
As	15.838	4.151	6.604	35.145	10.522	0.158	15.360	1.761	10.999	18.417	6.271	0.645
As^{+1}	15.023	3.255	7.473	22.587	9.509	0.028						
As^{+2}	14.424	2.145	9.068	14.857	7.457	0.023						
As^{+3}	16.605	1.024	10.974	10.360	2.424	0.015						
Se	16.322	4.144	6.708	35.224	10.932	0.154	15.856	1.752	11.244	18.303	6.515	0.644
Br	16.754	4.112	6.854	35.038	11.314	0.151	16.339	1.740	11.505	18.174	6.763	0.641
Kr	17.267	4.084	6.994	34.903	11.702	0.153	16.823	1.732	11.759	18.061	7.017	0.633
Rb	17.724	4.073	7.116	34.766	12.118	0.154	17.317	1.723	12.005	17.974	7.257	0.633
Rb^{+1}	16.926	3.303	7.950	23.088	11.129	0.023						
Sr	18.196	4.068	7.222	34.757	12.540	0.153	17.790	1.712	12.272	17.827	7.516	0.630
Y	18.666	4.067	7.315	34.842	12.976	0.154	18.275	1.700	12.523	17.687	7.764	0.625
Zr	19.128	4.033	7.466	34.563	13.361	0.155	18.776	1.695	12.754	17.633	8.027	0.619
Zr^{+4}	22.716	0.7120	13.535	8.695	-0.2475	0.010						
Nb	19.604	4.028	7.563	34.636	13.739	0.153	19.243	1.683	13.019	17.472	8.280	0.620
Mo	20.052	3.934	7.719	34.363	14.180	0.152	19.732	1.675	13.253	17.354	8.537	0.614
Mo^{+1}	19.255	3.315	8.545	23.535	13.165	0.027						
Tc	20.520	4.009	7.782	34.514	14.548	0.154	20.216	1.667	13.503	17.277	8.797	0.610
Ru	21.003	3.994	7.886	34.506	15.062	0.157	20.694	1.656	13.762	17.144	9.052	0.610
Rh	21.446	3.957	8.049	34.203	15.452	0.153	21.194	1.652	13.982	17.107	9.325	0.605
Pd	21.934	3.957	8.122	34.370	15.893	0.149	21.683	1.644	14.220	17.004	9.586	0.605
Ag	22.368	3.933	8.268	34.120	16.312	0.148	22.171	1.638	14.453	16.945	9.860	0.598
Ag^{+1}	21.643	3.294	9.164	23.747	15.196	0.030						
Cd	22.825	3.935	8.344	34.125	16.773	0.152	22.652	1.629	14.692	16.832	10.125	0.594
In	23.299	3.905	8.479	33.954	17.162	0.149	23.146	1.624	14.915	16.760	10.398	0.592
Sn	23.762	3.904	8.572	33.992	17.603	0.148	23.628	1.618	15.150	16.682	10.673	0.591
Sb	24.199	3.894	8.685	33.872	18.057	0.150	24.117	1.610	15.384	16.608	10.943	0.585
Te	24.677	3.884	8.770	33.904	18.495	0.146	24.594	1.603	15.626	16.493	11.214	0.585
I	25.122	3.871	8.881	33.759	18.934	0.145	25.080	1.597	15.854	16.420	11.487	0.580
Xe	25.583	3.853	8.993	33.730	19.361	0.144	25.578	1.590	16.073	16.367	11.761	0.579
Cs	26.033	3.842	9.097	33.634	19.804	0.146	26.069	1.587	16.286	16.309	12.048	0.575
Ba	26.491	3.834	9.195	33.604	20.249	0.144	26.534	1.579	16.532	16.213	12.327	0.574
La	26.939	3.825	9.291	33.579	20.705	0.145	27.052	1.577	16.721	16.207	12.616	0.570
Ce	27.382	3.814	9.399	33.529	21.154	0.143	27.529	1.569	16.952	16.118	12.837	0.569
Pr	27.833	3.807	9.487	33.462	21.611	0.143	28.009	1.562	17.188	16.033	13.169	0.563
Nd	28.296	3.805	9.560	33.496	22.074	0.143	28.493	1.557	17.408	15.956	13.452	0.562
Pm	28.749	3.794	9.659	33.471	22.521	0.140	28.990	1.554	17.612	15.932	13.745	0.561
Sm	29.196	3.769	9.794	33.248	22.935	0.141	29.467	1.547	17.843	15.843	14.028	0.557
Eu	29.642	3.758	9.894	33.212	23.390	0.140	29.959	1.543	18.044	15.806	14.317	0.554
Gd	30.074	3.757	9.980	33.140	23.872	0.139	30.436	1.535	18.290	15.713	14.596	0.551
Tb	30.525	3.739	10.092	33.050	24.308	0.140	30.930	1.532	18.491	15.675	14.893	0.548
Dy	30.985	3.733	10.169	33.072	24.770	0.137	31.421	1.528	18.697	15.619	15.187	0.548
Ho	31.430	3.723	10.271	32.591	23.222	0.137	31.902	1.523	18.915	15.565	15.480	0.544
Er	31.886	3.716	10.351	32.577	25.686	0.138	32.378	1.513	19.135	15.489	15.773	0.543
Tm	32.319	3.706	10.446	32.537	26.152	0.139	32.869	1.514	19.335	15.442	16.069	0.539
Yb	32.754	3.693	10.550	32.542	26.603	0.133	33.356	1.509	19.540	15.402	16.350	0.533
Lu	33.203	3.687	10.557	32.500	27.076	0.136	33.853	1.504	19.750	15.332	16.635	0.535

Table 2 (*cont.*)

Element	CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
	A	a	B	b	C	c	A	a	B	b	C	c
Hf	33.650	3.678	10.727	32.737	27.537	0.135	34.348	1.501	19.947	15.318	16.558	0.534
Ta	34.087	3.671	10.816	32.661	28.008	0.136	34.811	1.496	20.179	15.232	17.252	0.530
W	34.536	3.660	10.909	32.607	28.455	0.136	35.302	1.491	20.324	15.181	17.545	0.528
Re	34.969	3.652	11.004	32.564	28.937	0.134	35.784	1.487	20.591	15.139	17.849	0.527
Os	35.409	3.656	11.054	32.638	29.448	0.134	36.271	1.482	20.797	15.085	18.145	0.525
Ir	35.859	3.631	11.190	32.440	29.860	0.133	36.758	1.480	20.932	15.049	18.458	0.523
Pt	36.300	3.626	11.257	32.440	30.340	0.133	37.245	1.475	21.198	14.999	18.756	0.521
Au	36.729	3.611	11.383	32.280	30.794	0.132	37.724	1.472	21.399	14.961	19.070	0.518
Au^{+}	36.197	3.200	12.339	24.720	29.454	0.041						
Hg	37.156	3.612	11.444	32.315	31.304	0.132	38.124	1.469	21.624	14.878	19.431	0.532
Hg^{2+}	36.104	2.715	13.921	18.924	27.924	0.009						
Tl	37.593	3.615	11.488	32.416	31.822	0.132	38.683	1.462	21.809	14.836	19.680	0.514
Tl^{+1}	37.059	3.186	12.553	24.652	30.375	0.044						
Tl^{+3}	36.339	2.178	16.088	14.748	25.585	0.012						
Pb	38.034	3.590	11.629	32.214	32.238	0.132	39.023	1.461	22.052	14.757	20.078	0.538
Pb^{+3}	36.749	2.178	16.238	14.746	25.022	0.009						
Bi	38.461	3.599	11.671	32.314	32.773	0.132	39.761	1.538	21.490	15.420	20.974	0.462
Po	38.891	3.585	11.776	32.170	33.235	0.130	40.136	1.452	22.407	14.736	20.610	0.509
At	39.319	3.586	11.836	32.208	33.747	0.131	40.621	1.448	22.508	14.695	20.915	0.506
Rn	39.764	3.575	11.927	32.157	34.211	0.129	41.111	1.445	22.800	14.655	21.224	0.506
Fr	40.189	3.564	12.030	32.043	34.650	0.129	41.590	1.442	22.937	14.622	21.543	0.502
Ra	40.625	3.556	12.114	32.006	35.158	0.130	42.026	1.439	23.176	14.595	21.839	0.500
Ac	41.071	3.545	12.204	31.952	35.622	0.123	42.562	1.434	23.389	14.539	22.161	0.501
Th	41.483	3.542	12.283	31.889	36.130	0.123	43.042	1.430	23.533	14.495	22.471	0.497
Pa	41.915	3.534	12.365	31.875	36.613	0.126	43.534	1.428	23.758	14.475	22.795	0.496
U	42.362	3.525	12.450	31.845	37.081	0.125	44.011	1.425	23.952	14.434	23.115	0.495
Np	42.775	3.525	12.516	31.732	37.601	0.127	44.495	1.422	24.160	14.392	23.426	0.492
Pu	43.217	3.520	12.578	31.843	38.035	0.127	44.985	1.419	24.336	14.364	23.751	0.491
Am	43.646	3.511	12.671	31.745	38.571	0.127	45.461	1.416	24.535	14.321	24.068	0.489
Cm	44.093	3.499	12.753	31.721	39.036	0.123	45.952	1.413	24.715	14.255	24.391	0.489
Bk	44.505	3.501	12.819	31.744	39.563	0.123	46.438	1.410	24.907	14.263	24.707	0.487
Cf	44.939	3.492	12.901	31.693	40.048	0.125	46.930	1.408	25.076	14.240	25.038	0.484
Es	45.342	3.487	12.952	31.583	40.552	0.123	47.394	1.404	25.295	14.198	25.347	0.483
Fm	45.789	3.477	13.071	31.581	41.026	0.123	47.887	1.402	25.464	14.167	25.677	0.482
Md	46.200	3.475	13.144	31.544	41.541	0.123	48.367	1.398	25.659	14.133	25.996	0.479
No	46.630	3.465	13.229	31.467	42.022	0.123	48.855	1.396	25.834	14.102	26.326	0.478
Lr	47.052	3.460	13.304	31.442	42.526	0.121	49.340	1.393	26.023	14.071	26.644	0.475
– 104	47.484	3.452	13.387	31.394	43.013	0.121	49.822	1.391	26.204	14.041	26.977	0.475

Table 3. *Correspondence between theoretical and least-squares atomic scattering factors*

$\sin\theta/\lambda$		0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7
f (theoretical)		28·00	27·53	26·19	24·17	21·74	19·17	16·68	14·42
f (least squares)	$\varepsilon=0·01$	28·00	27·53	26·19	24·17	21·74	19·17	16·68	14·42
	$\varepsilon=0·09$	28·00	27·53	26·20	24·20	21·78	19·21	16·71	14·45
	$\varepsilon=1·01$	28·00	27·53	26·22	24·26	21·94	19·51	17·20	15·12

Appendix G

Coherent Neutron Scattering Amplitudes (compiled February, 1971, M. I. T.)

All amplitudes are of positive sign unless otherwise noted and are in units of 10^{-12} cm per atom.
Complex amplitudes correspond to a neutron wavelength of 1 Å.
Numbers in parenthesis are standard errors for entries of higher precision. For such, the values are representative of nuclear scattering only and do not include the neutron-electronic charge (Foldy) contribution.

Z	Element or Isotope	b_{coh}
1	H	-0.3723(3)
	D	0.670(5)
	H^3	0.47
2	He^4	0.30
3	Li	-0.194
	Li^6	0.18+0.025i
	Li^7	-0.21
4	Be	0.774
5	B	0.54+0.021i
	B^{11}	0.60
6	C	0.6626(3)
	C^{13}	0.60
7	N	0.940
8	O	0.575(4)
	O^{17}	0.578
	O^{18}	0.600
9	F	0.574(4)
10	Ne	0.46
11	Na	0.351
12	Mg	0.516
13	Al	0.3449(9)
14	Si	0.4151(1)
15	P	0.51
16	S	0.2847(1)
17	Cl	0.9584(2)
	Cl^{35}	1.18
	Cl^{37}	0.26
18	A	0.20
	A^{36}	2.43
19	K	0.37
	K^{39}	0.37
20	Ca	0.49
	Ca^{40}	0.49
	Ca^{44}	0.18
21	Sc	1.18
22	Ti	-0.33
	Ti^{46}	0.48
	Ti^{47}	0.33
	Ti^{48}	-0.58
	Ti^{49}	0.08
	Ti^{50}	0.55
23	V	-0.048
24	Cr	0.3532(10)
	Cr^{52}	0.490
25	Mn	-0.36
26	Fe	0.951
	Fe^{54}	0.42
	Fe^{56}	1.01
	Fe^{57}	0.23
27	Co	0.250
28	Ni	1.03
	Ni^{58}	1.44
	Ni^{60}	0.282
	Ni^{61}	0.76
	Ni^{62}	-0.87
	Ni^{64}	-0.037
29	Cu	0.76
	Cu^{63}	0.67
	Cu^{65}	1.11
30	Zn	0.57
	Zn^{64}	0.56
	Zn^{66}	0.63
	Zn^{68}	0.67
31	Ga	0.72
32	Ge	0.84
33	As	0.64
34	Se	0.78
35	Br	0.685(4)
36	Kr	0.74
37	Rb	0.85
	Rb^{85}	0.83
38	Sr	0.656
39	Y	0.79
40	Zr	0.69
41	Nb	0.711(4)
42	Mo	0.66
43	Tc^{99}	0.68
44	Ru	0.73
45	Rh	0.59
46	Pd	0.60
47	Ag	0.61
	Ag^{107}	0.83
	Ag^{109}	0.43
48	Cd	0.37+0.16i
	Cd^{113}	-1.5+1.2i
49	In	0.39
50	Sn	0.61
	Sn^{116}	0.58
	Sn^{117}	0.64
	Sn^{118}	0.58
	Sn^{119}	0.60
	Sn^{120}	0.64
	Sn^{122}	0.55
	Sn^{124}	0.59
51	Sb	0.5641(12)
52	Te	0.543(4)
	Te^{120}	0.52
	Te^{123}	0.57
	Te^{124}	0.55
	Te^{125}	0.56
53	I	0.52
54	Xe	0.480
55	Cs	0.55
56	Ba	0.52
57	La	0.83
58	Ce	0.46
	Ce^{140}	0.47
	Ce^{142}	0.45
59	Pr	0.44
60	Nd	0.72
	Nd^{142}	0.77
	Nd^{144}	0.28
	Nd^{146}	0.87
62	Sm^{152}	-0.5
	Sm^{154}	0.8
63	Eu	0.55
64	Gd	1.5
65	Tb	0.76
66	Dy	1.69
	Dy^{160}	0.67
	Dy^{161}	1.03
	Dy^{162}	-0.14
	Dy^{163}	0.50
	Dy^{164}	4.94
67	Ho	0.85
68	Er	0.79
69	Tm	0.69
70	Yb	1.26
71	Lu	0.73
72	Hf	0.73
73	Ta	0.691(7)
74	W	0.477(5)
	W^{182}	0.333(14)
	W^{183}	0.43(5)
	W^{184}	0.759(9)
	W^{186}	-0.119(5)
75	Re	0.92
76	Os	1.07
	Os^{188}	0.78
	Os^{189}	1.10
	Os^{190}	1.14
	Os^{192}	1.19
77	Ir	1.06
78	Pt	0.95
79	Au	0.76
80	Hg	1.266(2)
81	Tl	0.89
82	Pb	0.9404(4)
83	Bi	0.8525(5)
90	Th	0.99
92	U	0.85
	U^{235}	0.98
	U^{238}	0.85
93	Np	1.055
94	Pu	0.75

A P P E N D I X E

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              PROGRAM POWPAT(INPUT,OUTPUT)                                      POWPAT      2
        C     INTENSITY CALCULATION FOR POWDER DIFFRACTION PATTERNS             POWPAT      3
        C                          (1969 VERSION)                               POWPAT      4
        C     PROGRAM WRITTEN BY K.YVON, W.JEITSCHKO AND E.PARTHE               POWPAT      5
        C        SCHOOL OF METALLURGY AND MATERIALS SCIENCE                     POWPAT      6
        C     LABORATORY FOR RESEARCH ON THE STRUCTURE OF MATTER                POWPAT      7
        C       UNIVERSITY OF PENNSYLVANIA, PHILADELPHIA 19104                  POWPAT      8
000003        DIMENSION Q(3000),YH(3000),YK(3000),YL(3000),THETA(3000),SUMA(3000 POWPAT      9
             1),SUMB(3000),VINT(3000),NA(8),X(48,8),Y(48,8),Z(48,8),AAA(8),AA(8) POWPAT     10
             2,BBB(8),BB(8),CCC(8),BTEMP(8),ELEMT(8),PLAY(100),COMPND(20),SP(180 POWPAT     11
             3),W(180),FOCCU(8),STRU(3000),SFA(30,8),FPLG(3000),FMUL(3000)      POWPAT     12
000003   7000 FORMAT(/27H1INTENSITY CALCULATION FOR ,20A4/)                     POWPAT     13
000003   7001 FORMAT(/25H1DIFFRACTION PATTERN FOR ,20A4,4H WL=,F8.5/)           POWPAT     14
000003   7008 FORMAT (5X,15F5.0)                                                POWPAT     15
000003   7009 FORMAT(15F5.0)                                                    POWPAT     16
000003   7010 FORMAT(A4,F6.0,6F10.0)                                            POWPAT     17
000003   7011 FORMAT(/46H COEFFICIENTS FOR ATOMIC SCATTERING FACTOR OF A4,5F10.4 POWPAT     18
             1,/7H BTEMP=F10.5,58H ,OCCUPATION FACTOR (FOCCU) OF THE FOLLOWING P POWPAT     19
             2OSITIONS IS F10.5,/)                                              POWPAT     20
000003   7012 FORMAT(/23H SCATTERING FACTORS OF A4, 34H IN STEPS OF .05*SIN(THET POWPAT     21
             1A)/LAMBDA,/ 0P15F7.3,/ 0P15F7.3,//7H BTEMP=F10.5,58H ,OCCUPATION F POWPAT     22
             2ACTOR (FOCCU) OF THE FOLLOWING POSITIONS IS F10.5,8X,/)           POWPAT     23
000003   7020 FORMAT(3F10.0)                                                    POWPAT     24
000003   7021 FORMAT(1X,A4,1X,3F10.5)                                           POWPAT     25
000003   7022 FORMAT(1X,A4,1X,3F10.5,17H   +(1/2 1/2 1/2))                      POWPAT     26
000003   7023 FORMAT(1X,A4,1X,3F10.5,29H   +(2/3 1/3 1/3,1/3 2/3 2/3))          POWPAT     27
000003   7024 FORMAT(1X,A4,1X,3F10.5,35H   +(1/2 1/2 0,1/2 0 1/2,0 1/2 1/2))    POWPAT     28
000003   7025 FORMAT(1X,A4,1X,3F10.5,15H   +(0 1/2 1/2))                        POWPAT     29
000003   7026 FORMAT(1X,A4,1X,3F10.5,15H   +(1/2 0 1/2))                        POWPAT     30
000003   7027 FORMAT(1X,A4,1X,3F10.5,15H   +(1/2 1/2 0))                        POWPAT     31
000003   7049 FORMAT(10X,'   ATOMS IN UNIT CELL: ELEMT(M)  NA(M)*NBRA*FOCCU(M)') POWPAT     32
000003   7050 FORMAT(35X,A4,5X,I2,3H  *,I2,3H  *,F6.2)                          POWPAT     33
000003   7052 FORMAT (F8.1,4X,100A1)                                            POWPAT     34
000003   8001 FORMAT(3H A=F9.5,3H,B=F9.5,3H,C=F9.5,6H,BETA=F9.5,4H,WL=F8.5)     POWPAT     35
000003   8002 FORMAT(3H A=F9.5,3H,B=F9.5,3H,C=F9.5,4H,WL=F8.5,9H ANGSTROM)      POWPAT     36
000003   8003 FORMAT(3H A=F9.5,3H,C=F9.5,4H,WL=F8.5,9H ANGSTROM)                POWPAT     37
000003   8005 FORMAT(3H A=F9.5, 4H,WL=F8.5,9H ANGSTROM)                         POWPAT     38
000003   8007 FORMAT(3H A=F9.5,3H,B=F9.5,3H,C=F9.5,7H,ALPHA=F9.5,6H,BETA=F9.5,7H POWPAT     39
             1,GAMMA=F9.5,4H,WL=F8.5)                                           POWPAT     40
000003   8010 FORMAT(48H  SIN-SQUARE-THETA-VALUES CALCULATED BETWEEN SL=F7.4,8H  POWPAT     41
             1AND SH=F7.4,9X,6HKODLP=,I2,9X,6HAGUIN=0PF5.2,6X,6HBGUIN=0PF5.2)   POWPAT     42
000003   8011 FORMAT(38H DATA CALCULATED FOR LOW LAUE-SYMMETRY)                 POWPAT     43
000003   8012 FORMAT(39H DATA CALCULATED FOR HIGH LAUE-SYMMETRY)                POWPAT     44
000003   8029 FORMAT (20A4)                                                     POWPAT     45
000003   8031 FORMAT(39H SYMMETRY CENTER AT ORIGIN OF UNIT CELL)                POWPAT     46
000003   8842 FORMAT(19H HKO ONLY WITH H=2N)                                    POWPAT     47
000003   8843 FORMAT(19H HKO ONLY WITH K=2N)                                    POWPAT     48
000003   8844 FORMAT(19H HKO ONLY WITH H+K=I1,1HN)                              POWPAT     49
000003   8847 FORMAT (19H OKL ONLY WITH K=2N)                                   POWPAT     50
000003   8848 FORMAT(19H OKL ONLY WITH L=2N)                                    POWPAT     51
000003   8849 FORMAT(19H OKL ONLY WITH K+L=I1,1HN)                              POWPAT     52
000003   8852 FORMAT(19H HOL ONLY WITH H=2N)                                    POWPAT     53
000003   8853 FORMAT(19H HOL ONLY WITH L=2N)                                    POWPAT     54
000003   8854 FORMAT(19H HOL ONLY WITH H+L=I1,1HN)                              POWPAT     55
000003   8857 FORMAT(19H HHL ONLY WITH L=2N)                                    POWPAT     56
000003   8858 FORMAT(22H HHL ONLY WITH 2H+L=4N)                                 POWPAT     57
000003   8860 FORMAT(17H HOO ONLY WITH H=I1,1HN)                                POWPAT     58
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000003    8863 FORMAT(19H OKO ONLY WITH K=2N)                                    POWPAT    59
000003    8865 FORMAT(17H OOL ONLY WITH L=I1,1HN)                                POWPAT    60
000003    8881 FORMAT (49H PRIMITIVE BRAVAISLATTICE.ALL HKL VALUES ALLOWED )     POWPAT    61
000003    8882 FORMAT (51H BODYCENTERED BRAVAISLATTICE.HKL ONLY WITH H+K+L=2N)   POWPAT    62
000003    8883 FORMAT (52H RHOMBOHEDRAL BRAVAISLATTICE.HKL ONLY WITH -H+K+L=3N)  POWPAT    63
000003    8884 FORMAT (54H FACECENTERED BRAVAISLATTICE.H,K,L ALL EVEN OR ALL ODD) POWPAT    64
000003    8885 FORMAT (47H A-CENTERED BRAVAISLATTICE.HKL ONLY WITH K+L=2N)       POWPAT    65
000003    8886 FORMAT (47H B-CENTERED BRAVAISLATTICE.HKL ONLY WITH H+L=2N)       POWPAT    66
000003    8887 FORMAT (47H C-CENTERED BRAVAISLATTICE.HKL ONLY WITH H+K=2N)       POWPAT    67
000003    8990 FORMAT(/48H DATA CALCULATED FOR A MONOCLINIC STRUCTURE WITH)      POWPAT    68
000003    8991 FORMAT(/47H DATA CALCULATED FOR A TRICLINIC STRUCTURE WITH)       POWPAT    69
000003    8992 FORMAT(/51H DATA CALCULATED FOR AN ORTHORHOMBIC STRUCTURE WITH )  POWPAT    70
000003    8993 FORMAT(/50H DATA CALCULATED FOR A TRIGONAL STRUCTURE WITH      )  POWPAT    71
000003    8994 FORMAT (/48H DATA CALCULATED FOR A TETRAGONAL STRUCTURE WITH    )  POWPAT    72
000003    8995 FORMAT(/43H DATA CALCULATED FOR A CUBIC STRUCTURE WITH )          POWPAT    73
000003    8996 FORMAT (/47H DATA CALCULATED FOR A HEXAGONAL STRUCTURE WITH )     POWPAT    74
000003    8998 FORMAT( 130H1 H  K  L    THETA  SIN2*1000 INT.SCALED   INTENSITY U POWPAT    75
            1NSCALED          /F(HKL)/**2        A(HKL)        B(HKL) PHA.ANG. MU POWPAT    76
            2LT    LPG )                                                        POWPAT    77
000003    8999 FORMAT( 132H1 H  K  L  THETA  2THETA D-VALUE  SIN   SIN2*1000  H  POWPAT    78
            1K  L   INTENSITY      /F(HKL)/**2      A(HKL)     B(HKL) PHA.ANG.  POWPAT    79
            2MULT     LPG)                                                       POWPAT    80
000003    9900 FORMAT(21H SOMETHING WENT WRONG)                                  POWPAT    81
000003    9997 FORMAT(4I2,2X,7I2,6X,9I2)                                         POWPAT    82
000003    9998 FORMAT(F10.0,2F5.0,4I2,2X,2F10.0)                                 POWPAT    83
000003    9999 FORMAT(6F10.0)                                                    POWPAT    84
000003    9000 FORMAT(3I3,2F7.2, F8.4,2X,F6.4, 3PF9.2,1X,3I3,0PF11.1,0PF17.1,    POWPAT    85
            1 0P2F12.2,0PF8.3,0PF5.0,0PF9.2)                                     POWPAT    86
000003    9001 FORMAT(3I3,F9.2,3P1F10.2,0PF10.1,0PF22.1,0PF20.1,0P2F14.2,0PF8.3, POWPAT    87
            10PF5.0,0PF10.2)                                                     POWPAT    88
      C      SETCMA IS A ROUTINE THAT ALLOWS THE USE OF COMMAS ON INPUT          SETCMA     2
      C      AS SEPARATORS.  THIS AVOIDS THE NECESSITY OF SPACING TO             SETCMA     3
      C      A SPECIFIC COLUMN WHEN USING A TELETYPE.  THIS FEATURE CAN          SETCMA     4
      C      ALSO BE USED WITH CARD INPUT.  CONVENTIONAL INPUT FORMATS           SETCMA     5
      C      MAY STILL BE USED.                                                  SETCMA     6
      C      AFTER A CALL SETCMA(1) THE FEATURE MAY BE DISABLED BY               SETCMA     7
      C      CALL SETCMA(0)                                                      SETCMA     8
      C      FOR USE ON ANOTHER COMPUTER THAT DOES NOT OFFER THIS FEATURE        SETCMA     9
      C      THIS CALL SETCMA(1) MAY BE REMOVED OR A DUMMY ROUTINE SUPPLIED.     SETCMA    10
000003         CALL SETCMA(1)                                                    SETCMA    11
000005         PI2 = 6.2831853                                                   POWPAT    90
000007         E=2.7182818                                                       POWPAT    91
000010         FRTD=4./3.                                                        POWPAT    92
000012         READ 9997,NCALCS                                                  POWPAT    93
000017         DO 998 NCALC=1,NCALCS                                             POWPAT    94
000021         READ 8029,(COMPND(I),I=1,20)                                      POWPAT    95
000032         READ 9999, A,B,C,ALPHA,BETA,GAMMA                                 POWPAT    96
000052         READ 9998,WL,SL,SH,NORM,ISCAT,IMAGE,KODLP,AGUIN,BGUIN             POWPAT    97
000100         READ 9997,ISYSTM,IBRAVL,LAUE,ISYMCE,IHKO,IOKL,IHOL,IHHL,IHOO,IOKO, POWPAT    98
            1IOOL,NCOMPO,(NA(II),II=1,8)                                         POWPAT    99
000142         IF((SH.EQ.0.).OR.(SH.GT.0.999))SH=0.999                           POWPAT   100
000152         N=0                                                               POWPAT   101
000153         ICON=0                                                            POWPAT   102
000154         VMXINT=0.                                                         POWPAT   103
000155         NLINE=0                                                           POWPAT   104
000156     699 DO 700 M=1,NCOMPO                                                 POWPAT   105
000160         READ 7010,ELEMT(M),FOCCU(M),AAA(M),AA(M),BBB(M),BB(M),CCC(M),     POWPAT   106
            1BTEMP(M)                                                            POWPAT   107
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000203          IF(ISCAT.NE.0) READ 7008,(SFA(I,N),I=1,15)                      POWPAT   108
000220          IF(ISCAT.NE.0) READ 7009,    (SFA(I,M),I=16,30)                 POWPAT   109
000235          NL=NA(M)                                                        POWPAT   110
000237      700 READ 7020,(X(I,M),Y(I,M),Z(I,M),I=1,NL)                         POWPAT   111
000266          PRINT 7000, COMPND                                              POWPAT   112
000273          WLSQ4=WL**2/4.                                                  POWPAT   113
000276          ASTAR=WLSQ4/A**2                                                POWPAT   114
000300          IF((ISYSTM.EQ.1).OR.(ISYSTM.EQ.2).OR.(ISYSTM.EQ.7))             POWPAT   115
               1BSTAR=WLSQ4/B**2                                                POWPAT   116
000316          IF(ISYSTM.NE.5) CSTAR=WLSQ4/C**2                                POWPAT   117
000323          BET=BETA*PI2/360.                                               POWPAT   118
000326          SINB2=(SIN(BET))**2                                             POWPAT   119
000330          COSB=COS(BET)                                                   POWPAT   120
000333          IF(ISYSTM.NE.7)GO TO 201                                        POWPAT   121
000335          ALPH=ALPHA*PI2/360.                                             POWPAT   122
000337          GAMM=GAMMA*PI2/360.                                             POWPAT   123
000342          SV=(ALPH+BET+GAMM)/2.                                           POWPAT   124
000346          VOL=2.*A*B*C*SQRT(SIN(SV)*SIN(SV-ALPH)*SIN(SV-BET)*SIN(SV-GAMM)) POWPAT   125
000374          AST=(B*C*SIN(ALPH))/VOL                                         POWPAT   126
000402          BST=(A*C*SIN(BET))/VOL                                          POWPAT   127
000407          CST=(A*B*SIN(GAMM))/VOL                                         POWPAT   128
000414          COAST=(COSB*COS(GAMM)-COS(ALPH))/(SIN(BET)*SIN(GAMM))           POWPAT   129
000430          COBST=(COS(GAMM)*COS(ALPH)-COSB)/(SIN(GAMM)*SIN(ALPH))          POWPAT   130
000444          COGST=(COS(ALPH)*COSB-COS(GAMM))/(SIN(ALPH)*SIN(BET))           POWPAT   131
000460      201 ZH=0.                                                           POWPAT   132
000461          ZK = 0.                                                         POWPAT   133
000462          ZL=0.                                                           POWPAT   134
000463      100 ZH=ZH+1.                                                        POWPAT   135
000465          GO TO(1,2,3,4,5,6,7),ISYSTM                                     POWPAT   136
000500        1 ZHTEST=(2.0*A*SQRT(SH))/WL                                      POWPAT   137
000506          IF(ZH.LE.ZHTEST)GO TO 205                                       POWPAT   138
000510          ZH=0.                                                           POWPAT   139
000511          ZK=ZK+1.                                                        POWPAT   140
000513          ZKTEST=(2.0*B*SQRT(SH))/WL                                      POWPAT   141
000520          IF(ZK.LE.ZKTEST)GO TO 1                                         POWPAT   142
000522          ZK=0.                                                           POWPAT   143
000523          IF(ICON.EQ.0)GO TO 203                                          POWPAT   144
000524          ZL=ZL-1.                                                        POWPAT   145
000526          GO TO 204                                                       POWPAT   146
000526      203 ZL=ZL+1.                                                        POWPAT   147
000530      204 ZLTEST=(2.0*C*SQRT(SH))/WL                                      POWPAT   148
000536          IF(ABS(ZL).LE.ZLTEST)GO TO 1                                    POWPAT   149
000541          IF(ICON.EQ.1)GO TO 202                                          POWPAT   150
000543          ICON=1                                                          POWPAT   151
000544          GO TO 201                                                       POWPAT   152
000545      205 ATEST=ASTAR*ZH**2/SINB2+BSTAR*ZK**2+CSTAR*ZL**2/SINB2-WLSQ4*2.*ZH* POWPAT   153
               1ZL*COSB/(A*C*SINB2)                                             POWPAT   154
000567          IF(ATEST.GT.SH) GO TO 100                                       POWPAT   155
000572          IF((ICON.EQ.0).OR.((ZH.GT.0.9).AND.(ZL.LT.(-0.9))))GO TO 70     POWPAT   156
000605          GO TO 100                                                       POWPAT   157
000605      202 PRINT 8990                                                      POWPAT   158
000611          PRINT 8001,A,B,C,BETA,WL                                        POWPAT   159
000627          GO TO 23                                                        POWPAT   160
000630        2 ATEST=ASTAR*ZH**2+BSTAR*ZK**2+CSTAR*ZL**2                       POWPAT   161
000641          IF(ATEST.LE.SH)GO TO 70                                         POWPAT   162
000643          ZH=0.                                                           POWPAT   163
000644          ZK=ZK+1.                                                        POWPAT   164
000646          BTEST=BSTAR*ZK**2+CSTAR*ZL**2                                   POWPAT   165
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000652          IF (BTEST.LE.SH)GO TO 2                                         POWPAT    166
000654          ZK=0.                                                           POWPAT    167
000655          ZL=ZL+1.                                                        POWPAT    168
000657          CTEST=CSTAR*ZL**2                                               POWPAT    169
000661          IF(CTEST.LE.SH)GO TO 2                                          POWPAT    170
000663          PRINT 8992                                                      POWPAT    171
000666          PRINT 8002,A,B,C,WL                                             POWPAT    172
000702          GO TO 23                                                        POWPAT    173
000703        3 ATEST=FRTD*ASTAR*(ZH**2+ZH*ZK+ZK**2)+CSTAR*ZL**2                POWPAT    174
000715          IF((ZH.EQ.0.).AND.(ZL.EQ.0.))GO TO 100                          POWPAT    175
000722          IF(ATEST.LE.SH)GO TO 210                                        POWPAT    176
000724          ZH=0.                                                           POWPAT    177
000725          ZK=ZK+1.                                                        POWPAT    178
000727          BTEST=FRTD*ASTAR*ZK**2+CSTAR*ZL**2                              POWPAT    179
000733          IF (BTEST.LE.SH) GO TO 3                                        POWPAT    180
000736          ZK=0.                                                           POWPAT    181
000737          IF(ICON.EQ.0)GO TO 220                                          POWPAT    182
000740          ZL=ZL-1.                                                        POWPAT    183
000742          GO TO 221                                                       POWPAT    184
000742      220 ZL=ZL+1.                                                        POWPAT    185
000744      221 CTEST=CSTAR*ZL**2                                               POWPAT    186
000747          IF(CTEST.LE.SH)GO TO 3                                          POWPAT    187
000751          IF(ICON.EQ.1)GO TO 211                                          POWPAT    188
000753          ICON=1                                                          POWPAT    189
000754          GO TO 201                                                       POWPAT    190
000755      210 IF((ICON.EQ.0).OR.((ZL.LT.(-0.9)).AND.((ZH.NE.0.).AND.(ZK.NE.0.))) POWPAT    191
               1)GO TO 70                                                       POWPAT    192
000772          GO TO 100                                                       POWPAT    193
000772      211 PRINT 8993                                                      POWPAT    194
000776          GO TO 71                                                        POWPAT    195
000777        4 ATEST=ASTAR*(ZH**2+ZK**2)+CSTAR*ZL**2                           POWPAT    196
001005          IF(ATEST.LE.SH)GO TO 70                                         POWPAT    197
001007          ZH=ZK+1.                                                        POWPAT    198
001011          ZK=ZH                                                           POWPAT    199
001012          BTEST=ASTAR*2.*ZH**2+CSTAR*ZL**2                                POWPAT    200
001016          IF(BTEST.LE.SH)GO TO 4                                          POWPAT    201
001021          ZH=0.                                                           POWPAT    202
001022          ZK=0.                                                           POWPAT    203
001023          ZL=ZL+1.                                                        POWPAT    204
001025          CTEST=CSTAR*ZL**2                                               POWPAT    205
001027          IF(CTEST.LE.SH)GO TO 4                                          POWPAT    206
001031          PRINT 8994                                                      POWPAT    207
001034          GO TO 71                                                        POWPAT    208
001035        5 ATEST=ASTAR*(ZH**2+ZK**2+ZL**2)                                 POWPAT    209
001043          IF(ATEST.LE.SH)GO TO 70                                         POWPAT    210
001045          ZH=ZK+1.                                                        POWPAT    211
001047          ZK=ZH                                                           POWPAT    212
001050          BTEST=ASTAR*(2.*ZH**2+ZL**2)                                    POWPAT    213
001054          IF(BTEST.LE.SH)GO TO 5                                          POWPAT    214
001056          ZH=ZL+1.                                                        POWPAT    215
001060          ZK=ZH                                                           POWPAT    216
001061          ZL=ZH                                                           POWPAT    217
001062          CTEST=ASTAR*3.*ZH**2                                            POWPAT    218
001064          IF(CTEST.LE.SH)GO TO 5                                          POWPAT    219
001067          PRINT 8995                                                      POWPAT    220
001072          PRINT 8002,A,WL                                                 POWPAT    221
001102          GO TO 23                                                        POWPAT    222
001103        6 ATEST=FRTD*ASTAR*(ZH**2+ZH*ZK+ZK**2)+CSTAR*ZL**2                POWPAT    223
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001115          IF(ATEST.LE.SH)GO TO 70                                         POWPAT   224
001117          ZH=ZK+1.                                                        POWPAT   225
001121          ZK=ZH                                                           POWPAT   226
001122          BTEST=FRTD*ASTAR*3.*ZH**2+CSTAR*ZL**2                           POWPAT   227
001131          IF (BTEST.LE.SH)GO TO 6                                         POWPAT   228
001133          ZH=0.                                                           POWPAT   229
001134          ZK=0.                                                           POWPAT   230
001135          ZL=ZL+1.                                                        POWPAT   231
001137          CTEST=CSTAR*ZL**2                                               POWPAT   232
001141          IF(CTEST.LE.SH)GO TO 6                                          POWPAT   233
001143          PRINT 8996                                                      POWPAT   234
001146          GO TO 71                                                        POWPAT   235
001147        7 ZHTEST=(2.0*A*SQRT(SH))/WL                                      POWPAT   236
001155          IF(ZH.LE.ZHTEST) GO TO 206                                      POWPAT   237
001157          ZH=0.                                                           POWPAT   238
001160          IF(ICON.LT.2)GO TO 212                                          POWPAT   239
001162          ZK=ZK-1.                                                        POWPAT   240
001164          GO TO 213                                                       POWPAT   241
001165      212 ZK=ZK+1.                                                        POWPAT   242
001167      213 ZKTEST=(2.0*B*SQRT(SH))/WL                                      POWPAT   243
001175          IF(ABS(ZK).LE.ZKTEST) GO TO 7                                   POWPAT   244
001200          ZK=0.                                                           POWPAT   245
001201          IF((ICON.EQ.0).OR.(ICON.EQ.2))GO TO 208                         POWPAT   246
001207          ZL=ZL-1.                                                        POWPAT   247
001211          GO TO 209                                                       POWPAT   248
001211      208 ZL=ZL+1.                                                        POWPAT   249
001213      209 ZLTEST=(2.0*C*SQRT(SH))/WL                                      POWPAT   250
001221          IF(ABS(ZL).LE.ZLTEST)GO TO 7                                    POWPAT   251
001224          ICON=ICON+1                                                     POWPAT   252
001226          GO TO (201,201,201,207),ICON                                    POWPAT   253
001235      206 ATEST=WLSQ4*((ZH*AST)**2+(ZK*BST)**2+(ZL*CST)**2+2.*ZK*ZL*BST*CST* POWPAT   254
               1COAST+2.*ZH*ZL*AST*CST*COBST+2.*ZH*ZK*AST*BST*COGST)            POWPAT   255
001267          IF(ATEST.GT.SH) GO TO 100                                       POWPAT   256
001272          IF(ICON.EQ.0) GO TO 70                                          POWPAT   257
001273          IF(((ZH.EQ.0.).AND.(ZK.EQ.0.)).OR.((ZK.EQ.0.).AND.(ZL.EQ.0.)).OR. POWPAT   258
               1((ZH.EQ.0.).AND.(ZL.EQ.0.)))GO TO 100                           POWPAT   259
001316          IF((ICON.EQ.1).AND.(ZL.LT.(-0.9)))GO TO 70                      POWPAT   260
001326          IF(((ICON.EQ.2).AND.(ZK.LT.(-0.9))).AND.(ZH.GT.0.9))GO TO 70    POWPAT   261
001342          IF((ICON.EQ.3).AND.((ZH*ZK*ZL).NE.0.))GO TO 70                  POWPAT   262
001352          GO TO 100                                                       POWPAT   263
001352      207 PRINT 8991                                                      POWPAT   264
001356          PRINT 8007,A,B,C,ALPHA,BETA,GAMMA,WL                            POWPAT   265
001400          GO TO 23                                                        POWPAT   266
001401       70 IF(ATEST.LT.SL) GO TO 100                                       POWPAT   267
001404          XH=ZH                                                           POWPAT   268
001405          XK=ZK                                                           POWPAT   269
001407          XL=ZL                                                           POWPAT   270
001410      171 GO TO (90,82,83,84,85,86,87),IBRAVL                             POWPAT   271
001423       82 TESTBR=(XH+XK+XL)/2.                                            POWPAT   272
001427          GO TO 89                                                        POWPAT   273
001430       83 TESTBR=(-XH+XK+XL)/3.                                           POWPAT   274
001434          GO TO 89                                                        POWPAT   275
001435       84 FACEHK=(XH+XK)/2.                                               POWPAT   276
001440          IF((AINT(FACEHK)-FACEHK).NE.0.)GO TO 100                        POWPAT   277
001443       85 TESTBR=(XK+XL)/2.                                               POWPAT   278
001446          GO TO 89                                                        POWPAT   279
001447       86 TESTBR=(XH+XL)/2.                                               POWPAT   280
001452          GO TO 89                                                        POWPAT   281
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001453      87 TESTBR=(XH+XK)/2.                                                POWPAT   282
001456      89 IF((AINT(TESTBR)-TESTBR).NE.0.)GO TO 100                         POWPAT   283
001461      90 IF(XL.EQ.0.)GO TO (91,105,104,105,102),IHKO                      POWPAT   284
001473      91 IF(XH.EQ.0.)GO TO (92,111,110,111,108),IOKL                      POWPAT   285
001505      92 IF(XK.EQ.0.)GO TO (93,117,116,117,114),IHOL                      POWPAT   286
001517      93 IF(XH.EQ.XK)GO TO (94,120,122),IHHL                              POWPAT   287
001530         IF((XK.EQ.XL).AND.(ISYSTM.EQ.5))GO TO (94,1201,1221),IHHL        POWPAT   288
001547      94 IF(XK.EQ.0..AND.XL.EQ.0.)GO TO (95,124,610,124),IHOO             POWPAT   289
001565      95 IF(XH.EQ.0..AND.XL.EQ.0.)GO TO (96,128),IOKO                     POWPAT   290
001601      96 IF(XH.EQ.0..AND.XK.EQ.0.)GO TO (170,130,130,130,610,130),IOOL    POWPAT   291
001621         GO TO 170                                                        POWPAT   292
001622     102 FIHKO=XH/2.                                                      POWPAT   293
001624     103 IF(AINT(FIHKO)-FIHKO)100,91,100                                  POWPAT   294
001627     104 FIHKO=XK/2.                                                      POWPAT   295
001631         GO TO 103                                                        POWPAT   296
001632     105 HKO=IHKO                                                         POWPAT   297
001634         FIHKO=(XH+XK)/HKO                                                POWPAT   298
001637         GO TO 103                                                        POWPAT   299
001637     108 FIOKL=XK/2.                                                      POWPAT   300
001641     109 IF(AINT(FIOKL)-FIOKL)100,92,100                                  POWPAT   301
001644     110 FIOKL=XL/2.                                                      POWPAT   302
001646         GO TO 109                                                        POWPAT   303
001647     111 OKL=IOKL                                                         POWPAT   304
001651         FIOKL=(XK+XL)/OKL                                                POWPAT   305
001654         GO TO 109                                                        POWPAT   306
001654     114 FIHOL=XH/2.                                                      POWPAT   307
001656     115 IF(AINT(FIHOL)-FIHOL)100,93,100                                  POWPAT   308
001661     116 FIHOL=XL/2.                                                      POWPAT   309
001663         GO TO 115                                                        POWPAT   310
001664     117 HOL=IHOL                                                         POWPAT   311
001666         FIHOL=(XH+XL)/HOL                                                POWPAT   312
001671         GO TO 115                                                        POWPAT   313
001671     120 FIHHL=XL/2.                                                      POWPAT   314
001673     121 IF(AINT(FIHHL)-FIHHL)100,96,100                                  POWPAT   315
001676     122 FIHHL=(2.*XH+XL)/4.                                              POWPAT   316
001702         GO TO 121                                                        POWPAT   317
001702    1201 FIHHL=XH/2.                                                      POWPAT   318
001704         GO TO 121                                                        POWPAT   319
001705    1221 FIHHL=(2.*XL+XH)/4.                                              POWPAT   320
001711         GO TO 121                                                        POWPAT   321
001711     124 HOO=IHOO                                                         POWPAT   322
001713         FIHOO=XH/HOO                                                     POWPAT   323
001714         IF(AINT(FIHOO)-FIHOO)100,95,100                                  POWPAT   324
001717     128 FIOKO=XK/2.                                                      POWPAT   325
001721         IF(AINT(FIOKO)-FIOKO)100,96,100                                  POWPAT   326
001724     130 OOL=IOOL                                                         POWPAT   327
001726         FIOOL=XL/OOL                                                     POWPAT   328
001727         IF((AINT(FIOOL)-FIOOL).NE.0.)GO TO 100                           POWPAT   329
001732     170 N=N+1                                                            POWPAT   330
001734         Q(N)=ATEST                                                       POWPAT   331
001736         YH(N)=XH                                                         POWPAT   332
001737         YK(N)=XK                                                         POWPAT   333
001741         YL(N)=XL                                                         POWPAT   334
001742         JJ=N                                                             POWPAT   335
001743         J=JJ-1                                                           POWPAT   336
001744         IF((LAUE.EQ.2).OR.(ZH.EQ.XK))GO TO 100                           POWPAT   337
001754         GO TO (100,100,100,724,725,724,100),ISYSTM                       POWPAT   338
001767     724 IF((ZH.GT.ZK).AND.(ZK.GT.0.))GO TO 731                           POWPAT   339
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002000          GO TO 100                                                       POWPAT    340
002000      725 IF((ZH.GT.ZK).AND.(ZK.GT.ZL))GO TO 731                          POWPAT    341
002012          GO TO 100                                                       POWPAT    342
002013      731 TEMP=XH                                                         POWPAT    343
002015          XH=XK                                                           POWPAT    344
002016          XK=TEMP                                                         POWPAT    345
002017          GO TO 171                                                       POWPAT    346
002017       71 PRINT 8003,A,C,WL                                               POWPAT    347
002031       23 PRINT 8010,SL,SH,KODLP,AGUIN,BGUIN                              POWPAT    348
002047          IF((ISYSTM.GT.3).AND.(ISYSTM.LT.7).AND.(LAUE.EQ.1))PRINT 8011   POWPAT    349
002071          IF((ISYSTM.GT.3).AND.(ISYSTM.LT.7).AND.(LAUE.EQ.2))PRINT 8012   POWPAT    350
002113          IF(IBRAVL.EQ.1)PRINT 8881                                       POWPAT    351
002121          IF(IBRAVL.EQ.2)PRINT 8882                                       POWPAT    352
002127          IF(IBRAVL.EQ.3)PRINT 8883                                       POWPAT    353
002135          IF(IBRAVL.EQ.4)PRINT 8884                                       POWPAT    354
002143          IF(IBRAVL.EQ.5)PRINT 8885                                       POWPAT    355
002151          IF(IBRAVL.EQ.6)PRINT 8886                                       POWPAT    356
002157          IF(IBRAVL.EQ.7)PRINT 8887                                       POWPAT    357
002165          IF((IHKO.EQ.2).OR.(IHKO.EQ.4))PRINT 8844,IHKO                   POWPAT    358
002203          IF(IHKO.EQ.3)PRINT 8843                                         POWPAT    359
002211          IF(IHKO.EQ.5)PRINT 8842                                         POWPAT    360
002217          IF((IOKL.EQ.2).OR.(IOKL.EQ.4))PRINT 8849,IOKL                   POWPAT    361
002235          IF(IOKL.EQ.3)PRINT 8848                                         POWPAT    362
002243          IF(IOKL.EQ.5)PRINT 8847                                         POWPAT    363
002251          IF((IHOL.EQ.2).OR.(IHOL.EQ.4))PRINT 8854,IHOL                   POWPAT    364
002267          IF(IHOL.EQ.3)PRINT 8853                                         POWPAT    365
002275          IF(IHOL.EQ.5)PRINT 8852                                         POWPAT    366
002303          IF(IHHL.EQ.2)PRINT 8857                                         POWPAT    367
002311          IF(IHHL.EQ.3)PRINT 8858                                         POWPAT    368
002317          IF(IHOO.NE.1)PRINT 8860,IHOO                                    POWPAT    369
002327          IF(IOKO.NE.1)PRINT 8863                                         POWPAT    370
002335          IF(IOOL.NE.1)PRINT 8865,IOOL                                    POWPAT    371
002345          IF(ISYMCE.EQ.1)PRINT 8031                                       POWPAT    372
002353       79 NBRA=IBRAVL                                                     POWPAT    373
002355          IF(IBRAVL.GT.4)NBRA=2                                           POWPAT    374
002360          PRINT 7049                                                      POWPAT    375
002364          DO 709 M=1,NCOMPO                                               POWPAT    376
002366          IF(FOCCU(M).EQ.0.)FOCCU(M)=1.0                                  POWPAT    377
002371      709 PRINT 7050,ELEMT(M),NA(M),NBRA,FOCCU(M)                         POWPAT    378
002410          FBRA=NBRA                                                       POWPAT    379
002411          DO 701 M=1,NCOMPO                                               POWPAT    380
002413          IF(ISCAT.EQ.0) PRINT 7011,ELEMT(M),AAA(M),AA(M),BBB(M),BB(M),   POWPAT    381
               1CCC(M),BTEMP(M),FOCCU(M)                                        POWPAT    382
002437          IF(ISCAT.NE.0)PRINT7012,ELEMT(M),(SFA(I,M),I=1,30),BTEMP(M),FOCCU( POWPAT  383
               1M)                                                              POWPAT    384
002462          NL=NA(M)                                                        POWPAT    385
002464          IF(IBRAVL.EQ.1) PRINT 7021,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  386
002515          IF(IBRAVL.EQ.2) PRINT 7022,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  387
002546          IF(IBRAVL.EQ.3) PRINT 7023,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  388
002577          IF(IBRAVL.EQ.4) PRINT 7024,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  389
002630          IF(IBRAVL.EQ.5) PRINT 7025,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  390
002661          IF(IBRAVL.EQ.6) PRINT 7026,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  391
002712      701 IF(IBRAVL.EQ.7) PRINT 7027,(ELEMT(M),X(I,M),Y(I,M),Z(I,M),I=1,NL) POWPAT  392
002746      750 DO 80 N=1,J                                                     POWPAT    393
002750          NN=N+1                                                          POWPAT    394
002752          DO 80 M=NN,JJ                                                   POWPAT    395
002754          IF((Q(N)-Q(M)).LE.0.)GO TO 80                                   POWPAT    396
002757          TEMP=Q(N)                                                       POWPAT    397
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002761          Q(N)=Q(M)                                                       POWPAT    398
002763          Q(M)=TEMP                                                       POWPAT    399
002764          TEMP=YH(N)                                                      POWPAT    400
002765          YH(N)=YH(M)                                                     POWPAT    401
002767          YH(M)=TEMP                                                      POWPAT    402
002771          TEMP=YK(M)                                                      POWPAT    403
002772          YK(N)=YK(M)                                                     POWPAT    404
002774          YK(M)=TEMP                                                      POWPAT    405
002775          TEMP=YL(N)                                                      POWPAT    406
002776          YL(N)=YL(M)                                                     POWPAT    407
003000          YL(M)=TEMP                                                      POWPAT    408
003002       80 CONTINUE                                                        POWPAT    409
003007          IF(NORM.EQ.1) PRINT 8999                                        POWPAT    410
003015          IF(NORM.NE.1)PRINT 8998                                         POWPAT    411
003023          AGUIN=AGUIN*PI2/360.                                            POWPAT    412
003026          DO 200 N=1,JJ                                                   POWPAT    413
003027          THETA(N)=57.29578*ATAN(SQRT(Q(N)/(1.-Q(N))))                    POWPAT    414
003041          VV=THETA(N)*0.0174533                                           POWPAT    415
003043          SX2=(SIN(VV)/WL)**2                                             POWPAT    416
003046          IF(KODLP.EQ.0) PLG=(1.+(1.-2.*Q(N))**2)/(Q(N)*SQRT(1.-Q(N)))    POWPAT    417
003064          IF(KODLP.EQ.1) PLG=1.                                           POWPAT    418
003070          IF(KODLP.EQ.2) PLG=1./(Q(N)*SQRT(1.-Q(N)))                      POWPAT    419
003102          IF(KODLP.EQ.3) PLG=(1.+((1.-2.*Q(N))**2)*((COS(AGUIN)))**2)/    POWPAT    420
               1(Q(N)*SQRT(1.-Q(N)))                                            POWPAT    421
003125          WW=(2.*THETA(N)-BGUIN)*0.0174533                                POWPAT    422
003132          IF(KODLP.EQ.4) PLG=(1.+((1.-2.*Q(N))**2)*((COS(AGUIN)))**2)/    POWPAT    423
               1((SQRT(Q(N)))*COS(WW)*SIN(2.*VV))                               POWPAT    424
003161          GO TO(501,502,503,504,505,506,602),ISYSTM                       POWPAT    425
003174      501 IF((YK(N).EQ.0.).OR.((YH(N).EQ.0.).AND.(YL(N).EQ.0.)))GO TO 602 POWPAT    426
003206      604 FMULTI=4.0                                                      POWPAT    427
003210          GO TO 530                                                       POWPAT    428
003210      502 IF(YH(N).EQ.0.)IF(YK(N))610,602,551                             POWPAT    429
003214          IF(YK(N).EQ.0.)GO TO 551                                        POWPAT    430
003216          IF(YL(N).EQ.0.) GO TO 604                                       POWPAT    431
003217      608 FMULTI=8.0                                                      POWPAT    432
003221          GO TO 530                                                       POWPAT    433
003221      551 IF(YL(N))610,602,604                                            POWPAT    434
003224      503 IF((YH(N).EQ.0.).AND.(YK(N).EQ.0.))GO TO 602                    POWPAT    435
003233      606 FMULTI=6.0                                                      POWPAT    436
003235          GO TO 530                                                       POWPAT    437
003235      504 IF((YH(N)-YK(N)).EQ.0.)IF(YH(M))610,602,552                     POWPAT    438
003242          IF(YK(N).EQ.0.)GO TO 552                                        POWPAT    439
003244          IF(YL(N).EQ.0.)IF(LAUE-1)610,604,608                            POWPAT    440
003250          IF(LAUE.EQ.1)GO TO 608                                          POWPAT    441
003252          FMULTI=16.                                                      POWPAT    442
003254          GO TO 530                                                       POWPAT    443
003254      552 IF(YL(N))610,604,608                                            POWPAT    444
003257      505 IF((YH(N)-YK(N)).EQ.0.) IF(YL(N))610,612,554                    POWPAT    445
003264          IF((YL(N).EQ.0.).AND.(LAUE.EQ.2))IF(YK(N)) 610,606,624          POWPAT    446
003276          IF((YL(N).EQ.0.).AND.(LAUE.EQ.1))IF(YK(N)) 610,606,612          POWPAT    447
003307          IF(((YK(N)-YL(N)).EQ.0.).OR.(LAUE.EQ.1)) GO TO 624              POWPAT    448
003317          FMULTI=48.                                                      POWPAT    449
003321          GO TO 530                                                       POWPAT    450
003321      554 IF(YH(N)-YL(N))610,608,624                                      POWPAT    451
003325      506 IF((YH(N)-YK(N)).EQ.0.)IF(YH(N))610,602,553                     POWPAT    452
003332          IF(YK(N).EQ.0.)GO TO 553                                        POWPAT    453
003334          IF((YL(N).EQ.0.).AND.(LAUE.EQ.1))GO TO 606                      POWPAT    454
003342          IF((YL(N).EQ.0.).OR.(LAUE.EQ.1)) GO TO 612                      POWPAT    455
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003351      624 FMULTI=24.0                                                   POWPAT    456
003353          GO TO 530                                                     POWPAT    457
003353      553 IF(YL(N))610,606,612                                          POWPAT    458
003356      602 FMULTI=2.0                                                    POWPAT    459
003360          GO TO 530                                                     POWPAT    460
003360      612 FMULTI=12.0                                                   POWPAT    461
003362      530 SUMA(N)=0.                                                    POWPAT    462
003364          SUMB(N)=0.                                                    POWPAT    463
003365          DO 703 M=1,NCOMPO                                             POWPAT    464
003366          SMA=0.                                                        POWPAT    465
003367          SMB=0.                                                        POWPAT    466
003370          NL=NA(M)                                                      POWPAT    467
003371          DO 704 I=1,NL                                                 POWPAT    468
003373          ARG=PI2*(YH(N)*X(I,M)+YK(N)*Y(I,M)+YL(N)*Z(I,M))              POWPAT    469
003410          SMA=SMA+COS(ARG)                                              POWPAT    470
003413          IF(ISYMCE.EQ.1)GO TO 704                                      POWPAT    471
003415          SMB=SMB+SIN(ARG)                                              POWPAT    472
003420      704 CONTINUE                                                      POWPAT    473
003423          FSCAT=AAA(M)*E**(-AA(M)*SX2)+BBB(M)*E**(-BB(M)*SX2)+CCC(M)    POWPAT    474
003442          IF(ISCAT.EQ.0)GO TO 702                                       POWPAT    475
003443          FL=(SQRT(SX2))/.05+1.0                                        POWPAT    476
003447          IFL=FL                                                        POWPAT    477
003451          FFL=FL-FLOAT(IFL)                                             POWPAT    478
003453          FSCAT=SFA(IFL,M)+(SFA(IFL+1,M)-SFA(IFL,M))*FFL                POWPAT    479
003462      702 FSMOD=FSCAT*FOCCU(M)*E**(-BTEMP(M)*SX2)                       POWPAT    480
003472          SUMA(N)=SUMA(N)+SMA*FSMOD                                     POWPAT    481
003476          SUMB(N)=SUMB(N)+SMB*FSMOD                                     POWPAT    482
003500      703 CONTINUE                                                      POWPAT    483
003503          SUMA(N)=FBRA*SUMA(N)                                          POWPAT    484
003505          SUMB(N)=FBRA*SUMB(N)                                          POWPAT    485
003507          FPLG(N)=PLG                                                   POWPAT    486
003510          FMUL(N)=FMULTI                                                POWPAT    487
003512          STRU(N)=SUMA(N)**2+SUMB(N)**2                                 POWPAT    488
003515          VINT(N)=PLG*FMULTI*STRU(N)                                    POWPAT    489
003520      200 VMXINT=AMAX1(VMXINT,VINT(N))                                  POWPAT    490
003525          DO 705 N=1,JJ                                                 POWPAT    491
003527      735 IH=YH(N)                                                      POWPAT    492
003532          IK=YK(N)                                                      POWPAT    493
003534          IL=YL(N)                                                      POWPAT    494
003536          DVAL=WL/(2.*SQRT(Q(N)))                                       POWPAT    495
003542          THETA2=2.*THETA(N)                                            POWPAT    496
003544          PRPINT=VINT(N)*1000./VMXINT                                   POWPAT    497
003546          VVV=Q(N)                                                      POWPAT    498
003550          SQURQ=(VVV)**0.5                                              POWPAT    499
003553          SUMAN=SUMA(N)                                                 POWPAT    500
003555          SUMBN=SUMB(N)                                                 POWPAT    501
003557          PHANG=0.0                                                     POWPAT    502
003560          IF((SUMAN.NE.0.).OR.(SUMBN.NE.0.))                            POWPAT    503
               1PHANG=(ATAN2(SUMBN,SUMAN))*360./PI2                           POWPAT    504
003573      712 NLINE=NLINE+1                                                 POWPAT    505
003575          IF(NLINE.NE.60)GO TO 711                                      POWPAT    506
003577          IF(NORM.EQ.1) PRINT 8999                                      POWPAT    507
003604          IF(NORM.NE.1) PRINT 8998                                      POWPAT    508
003612          NLINE=0                                                       POWPAT    509
003613      711 IF(NORM.EQ.1) GO TO 714                                       POWPAT    510
003615      713 PRINT 9001,IH,IK,IL,THETA(N),Q(N),PRPINT,VINT(N),STRU(N),SUMA(N),  POWPAT    511
               1SUMB(N),PHANG,FMUL(N),FPLG(N)                                 POWPAT    512
003653          GO TO 705                                                     POWPAT    513
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003654      714 PRINT 9000,IH,IK,IL,THETA(N),THETA2,DVAL,SQURQ,Q(N),IH,IK,IL,      POWPAT    514
               1PRPINT,STRU(N),SUMA(N),SUMB(N),PHANG,FMUL(N),FPLG(N)                POWPAT    515
003724      705 CONTINUE                                                            POWPAT    516
003727          IF(IMAGE.EQ.0)GO TO 998                                             POWPAT    517
003730          VMXINT=0.                                                           POWPAT    518
003731          PRINT 7001,COMPND,WL                                                POWPAT    519
003740          DATA STAR, BLANK/1H*,1H /                                           POWPAT    520
003740          W(1)=AINT(57.29578 * ATAN(SQRT(SL/(1.-SL))))                        POWPAT    521
003751          KK = (AINT(57.29578*ATAN(SQRT(SH/(1.-SH))))-W(1))*2.+1.             POWPAT    522
003766          DO 800 K=1,KK                                                       POWPAT    523
003767          SP(K)=0.                                                            POWPAT    524
003770          IF(K.NE.1) W(K) = W(K-1)+0.5                                        POWPAT    525
003774          DO 800 N=1,JJ                                                       POWPAT    526
003776          IF((THETA(N).GE.W(K)).AND.(THETA(N).LT.(W(K)+0.5))) SP(K)=SP(K)+    POWPAT    527
               1VINT(N)                                                             POWPAT    528
004014      800 VMXINT=AMAX1(VMXINT,SP(K))                                          POWPAT    529
004024          DO 804 K=1,KK                                                       POWPAT    530
004026          NSPIEL=(SP(K)*1000.)/(VMXINT*10.0)                                  POWPAT    531
004033          DO 802 MP=1,100                                                     POWPAT    532
004034      802 PLAY(MP)=BLANK                                                      POWPAT    533
004037          IF(NSPIEL.EQ.0) GO TO 804                                           POWPAT    534
004040          DO 803 MP=1,NSPIEL                                                  POWPAT    535
004042      803 PLAY(MP)=STAR                                                       POWPAT    536
004046      804 PRINT 7052,  W(K),(PLAY(MP),MP=1,NSPIEL)                            POWPAT    537
004066          GO TO 998                                                           POWPAT    538
004066      610 PRINT 9900                                                          POWPAT    539
004072      998 CONTINUE                                                            POWPAT    540
004075      997 CALL EXIT                                                           POWPAT    541
004076          END                                                                 POWPAT    542
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POWPAT

PROGRAM LENGTH INCLUDING I/O BUFFERS
113602

FUNCTION ASSIGNMENTS

STATEMENT ASSIGNMENTS

1	-	000500	2	-	000630	3	-	000703	4	-	000777
5	-	001035	6	-	001103	7	-	001147	23	-	002031
70	-	001401	71	-	002017	79	-	002353	80	-	003002
82	-	001423	83	-	001430	84	-	001435	85	-	001443
86	-	001447	87	-	001453	89	-	001456	90	-	001461
91	-	001473	92	-	001505	93	-	001517	94	-	001547
95	-	001565	96	-	001601	100	-	000463	102	-	001622
103	-	001624	104	-	001627	105	-	001632	108	-	001637
109	-	001641	110	-	001644	111	-	001647	114	-	001654
115	-	001656	116	-	001661	117	-	001664	120	-	001671
121	-	001673	122	-	001676	124	-	001711	128	-	001717
130	-	001724	170	-	001732	171	-	001410	201	-	000460
202	-	000605	203	-	000526	204	-	000530	205	-	000545
206	-	001235	207	-	001352	208	-	001211	209	-	001213
210	-	000755	211	-	000772	212	-	001165	213	-	001167
220	-	000742	221	-	000744	501	-	003174	502	-	003210
503	-	003224	504	-	003235	505	-	003257	506	-	003325
530	-	003362	551	-	003221	552	-	003254	553	-	003353

554	-	003321	602	-	003356	604	-	003206	606	-	003233
608	-	003217	610	-	004066	612	-	003360	624	-	003351
699	-	000156	701	-	002712	702	-	003462	704	-	003420
705	-	003724	709	-	002371	711	-	003613	712	-	003573
713	-	003615	714	-	003654	724	-	001767	725	-	002000
731	-	002013	735	-	003527	750	-	002746	800	-	004014
802	-	004034	803	-	004042	804	-	004046	997	-	004075
998	-	004072	1201	-	001702	1221	-	001705	7000	-	004106
7001	-	004114	7008	-	004123	7009	-	004126	7010	-	004130
7011	-	004133	7012	-	004153	7020	-	004177	7021	-	004201
7022	-	004204	7023	-	004211	7024	-	004220	7025	-	004227
7026	-	004234	7027	-	004241	7049	-	004246	7050	-	004256
7052	-	004263	8001	-	004266	8002	-	004275	8003	-	004304
8005	-	004312	8007	-	004317	8010	-	004331	8011	-	004347
8012	-	004355	8029	-	004363	8031	-	004365	8842	-	004373
8843	-	004377	8844	-	004403	8847	-	004410	8848	-	004414
8849	-	004420	8852	-	004425	8853	-	004431	8854	-	004435
8857	-	004442	8858	-	004446	8860	-	004452	8863	-	004456
8865	-	004462	8881	-	004466	8882	-	004475	8883	-	004504
8884	-	004513	8885	-	004523	8886	-	004532	8887	-	004541
8990	-	004550	8991	-	004557	8992	-	004566	8993	-	004575
8994	-	004604	8995	-	004613	8996	-	004622	8998	-	004631
8999	-	004650	9000	-	004706	9001	-	004721	9900	-	004670
9997	-	004674	9998	-	004700	9999	-	004704			

BLOCK NAMES AND LENGTHS

VARIABLE ASSIGNMENTS

A	-	111353	AA	-	066265	AAA	-	066255	AGUIN	-	111370
ALPH	-	111424	ALPHA	-	111356	ARG	-	111505	AST	-	111430
ASTAR	-	111416	ATEST	-	111444	B	-	111354	BB	-	066305
BBB	-	066275	BET	-	111421	BETA	-	111357	BGUIN	-	111371
BLANK	-	111527	BST	-	111431	BSTAR	-	111417	BTEMP	-	066325
BTEST	-	111445	C	-	111355	CCC	-	066315	COAST	-	111433
COBST	-	111434	COGST	-	111435	COMPND	-	066511	COSB	-	111423
CST	-	111432	CSTAR	-	111420	CTEST	-	111446	DVAL	-	111516
E	-	111346	ELEMT	-	066335	FACEHK	-	111453	FBRA	-	111474
FFL	-	111511	FIHHL	-	111462	FIHKO	-	111454	FIHOL	-	111460
FIHOO	-	111464	FIOKL	-	111456	FIOKO	-	111465	FIOOL	-	111467
FL	-	111507	FMUL	-	103455	FMULTI	-	111502	FOCCU	-	067305
FPLG	-	075565	FRTD	-	111347	FSCAT	-	111506	FSMOD	-	111512
GAMM	-	111425	GAMMA	-	111360	HKO	-	111455	HOL	-	111461
HOO	-	111463	I	-	111352	IBRAVL	-	111373	ICON	-	111410
IFL	-	111510	IH	-	111513	IHHL	-	111401	IHKO	-	111376
IHOL	-	111400	IHOO	-	111402	II	-	111406	IK	-	111514
IL	-	111515	IMAGE	-	111366	IOKL	-	111377	IOKO	-	111403
IOOL	-	111404	ISCAT	-	111365	ISYMCE	-	111375	ISYSTM	-	111372
J	-	111471	JJ	-	111470	K	-	111531	KK	-	111530
KODLP	-	111367	LAUE	-	111374	M	-	111413	MP	-	111533
N	-	111407	NA	-	064045	NBRA	-	111473	NCALC	-	111351
NCALCS	-	111350	NCOMPO	-	111405	NL	-	111414	NLINE	-	111412
NN	-	111475	NORM	-	111364	NSPIEL	-	111532	OKL	-	111457
OOL	-	111466	PHANG	-	111525	PI2	-	111345	PLAY	-	066345
PLG	-	111500	PRPINT	-	111520	Q	-	005145	SFA	-	075205
SH	-	111363	SINB2	-	111422	SL	-	111362	SMA	-	111503
SMB	-	111504	SP	-	066535	SQURQ	-	111522	STAR	-	111526
STRU	-	067315	SUMA	-	042375	SUMAN	-	111523	SUMB	-	050265
SUMBN	-	111524	SV	-	111426	SX2	-	111477	TEMP	-	111472

```
TESTBR - 111452    THETA  - 034505    THETA2 - 111517    VINT   - 056155
VMXINT - 111411    VOL    - 111427    VV     - 111476    VVV    - 111521
W      - 067021    WL     - 111361    WLSQ4  - 111415    WW     - 111501
X      - 064055    XH     - 111447    XK     - 111450    XL     - 111451
Y      - 064655    YH     - 013035    YK     - 020725    YL     - 026615
Z      - 065455    ZH     - 111436    ZHTEST - 111441    ZK     - 111437
ZKTEST - 111442    ZL     - 111440    ZLTEST - 111443

START OF CONSTANTS
004100

START OF TEMPORARIES
004776

START OF INDIRECTS
005123

UNUSED COMPILER SPACE
015700
```

NAME: PRJCTNC AUTHOR: L. Andrews

CORE: 37K DATE: October, 1973

PRØGRAM PRJCTN(INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT,PUNCH,TAPE1,TAPE2,TAPE3,
TAPE4,TAPE7=PUNCH)

I. PURPOSE:

Provide line drawings of molecules on CALCOMP with simple input and easy stereo rotation

II. TAPES:

TAPE1 unused
TAPE2 unused
TAPE3 input file from protein data bank, use BUPD140(C=TAPE3....)
TAPE4 CALCOMP output tape
TAPE5=INPUT
TAPE6=ØUTPUT
TAPE7=PUNCH

III. LIMITATIONS:

97 atoms
200 bonds
50 ATOM RANGE CARDS

IV. REPLACEABLE SUBROUTINES:

PRØTIN - library version gets protein main chain and hetero groups

CALCMP,QBLOCK,PLØTS,FIN, change to system versions if you want to use CRT

V. DECK SET UP

A. JOB CARD

1. TIME LIMIT - 17 sec
2. FIELD LENGTH - 37K
3. LINE LIMIT - 10K
4. NUMBER OF TAPES - 001
5. ECS - none

B. CONTROL CARDS

ØBTAIN(CPRØGS,CPRØGS,PRJCTNC)
REQUEST,TAPE4,5,Y,W,_____. NAME if you don't use TAPE NUMBER card.
PRJCTNC.
The request card is optional

C. DATA CARDS:

CARD	FORMAT
ATOM	A6,1X,A6,3F8.4
CELL	A6,1X,A6,3F8.4,3F9.5
STEREO	A10,F10.5,I10
DMAX	A10,F10.5
DMIN	A10,F10.5
TAPENUMBER	4A10
ATOMRANGE	A10,F10.5,4A10,2F10.5
FRAMESIZE	A10,2F10.5
SEPARATION	A10,F10.5
NORMAL	3A10
ATOMPLANE	3A10
PUNCH	A10
SCALE	A10,F10.5
PROTEIN	A10
CRT	A10
CHANGEPEN	A10

D. REMOTE FILES:

ØUTPUT (for checking bond lengths if desired)

PUNCH orthogonal Å coordinates

Brookhaven Crystallographic Computer Program

NAME: PRJCTNC TIME: <40 sec

CORE FL: $37K_8$

PRØGRAM PRJCTN(INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT,PUNCH,TAPE1,TAPE2,
TAPE3,TAPE4,TAPE7=PUNCH)

Provides a simple way to get line drawings of molecules. Current limits: 97 atoms, 200 bonds, 50 atom range cards. Symmetry generation is not provided. Below, **DEFAULT gives values assumed if card is missing. All card order is optional (DMAX and DMIN affect later ATOMRANGE cards).

Input:

A) Required Cards:

Card 1. ATOMS (min. 3, max. 97)

a) XRAY format (A6,1X,A6,3F8.4)

1-4	ATOM
8-13	Atom name
14-21	x in fractional coordinates
22-29	y in fractional coordinates
30-38	z in fractional coordinates

b) FLINUS format (A6,21X,3F9.6)

1-6	Atom Name
	x in fractional coordinates
	y in fractional coordinates
	z in fractional coordinates

N.B. Any card without a known identifier is assumed to be a FLINUS atom card!

B) Commonly used (but OPTIONAL) cards

Card 2. Cell (A6,7X,3F8.4,3F9.5)(XRAY format)

1-4	CELL
14-21	a
22-29	b
30-38	c

39-47 alpha or cos(alpha)

48-56 beta or cos(beta)

57-65 gamma or cos(gamma)

**DEFAULT--orthogonal 1.0 Angstrom cell, i.e. input coordinates in Angstroms

Card 3. Stereo (A10,F10.5,I10)

1-6 STEREO

11-20 degrees of rotation between views (0 gets 6 degrees)

21-30 number of views (0 gets 2 views, max = 50)

**DEFAULT--2 views, 6 degrees apart

Card 4. DMAX (A10,F10.5)

1-4 DMAX

11-20 maximum distance assumed to be bonded

**DEFAULT--1.7 A

Card 5. DMIN (A10,F10.5)

1-4 DMIN

11-20 minimum distance between atoms that will be drawn

**DEFAULT--0.0 A

Card 6. CALCOMP Tape Request (4A10)

1-10 TAPENUMBER

11-20 CSCF tape reel number

21-40 User name

**DEFAULT use a request card for TAPE4 (if this card is used, the request is not issued until the input has been checked).

C) Special Cards

Card 7. Special treatment at certain groups (A10,F10.5,4A10,2F10.5)

1-9 ATOMRANGE

11-20 Brightness for CRT (blank=16)

21-30 Beginning of first group

31-40 End of first group

41-50 Beginning of second group

51-60 End of second group

61-70 DMAX to apply to bonds between first group and second group

71-80 DMIN (like DMAX)

**DEFAULT--check each atom against every other atom in searching for bonds.

If an ATOMRANGE card is present, it is assumed that only bonds specified by atomrange cards are wanted. Only bonds between the two specified groups will be drawn. The groups may overlap. If only the first group is input, the second is assumed to be the same as the first. If the second atom at a group is absent, it is assumed to be the same as the first atom (i.e. a one atom group). If all four atom fields are blank, the card is assumed to apply to all atoms.

Card 8. Framesize (A10,2F10.5)

1-9 FRAMESIZE

11-20 Maximimum picture size along x (inches)

21-30 Maximum picture size along y (0.0 means same as x)

**DEFAULT--along x=2.0; along y=3.0

The views will fit inside boxes the size of the limits specified on the FRAMESIZE card (unless a SCALE card is included) (use 4.0 or 4.5 for large viewer)

Card 9. Picture Separation (A10,F10.5)

1-10 SEPARATION

11-20 distance between views (0.0 is allowed)

**DEFAULT--2.25 in (good for stereo vision) (use 9.2 for large viewer)

Card 10. Viewing angle (3A10)

1-6 NORMAL

11-20, 21-30 left adjusted names of two atoms which define a normal to the plane at the initial projection

**DEFAULT--the initial view will look at the x,y plane

Card 11. Viewing angle (4A10)

1-9 ATOMPLANE

11-20, 21-30, 31-40 left adjusted names of three atoms which define the plane at the initial projection

**DEFAULT--The initial view will look at the x,y plane

D) <u>Special Purpose Cards</u>

Card 12. Punched Orthogonal Angstrom Output (A10)

1-5 PUNCH

**DEFAULT--no punched output

Card 13. Picture scaling (A10,F10.5)

1-5 SCALE

11-20 Scale factor to multiply picture size

**DEFAULT--1.0

Card 14. Protein Data Bank main chain plots (A10)

1-7 PROTEIN

**DEFAULT--atomic parameters from INPUT.

a BCD PDB COMPILE file must be on TAPE3.

use BUPD140(C=TAPE3,...)

Card 15. Cathode Ray Tube Plots (A10)

1-3 CRT

**DEFAULT--mechanical plotter

(N.B. not checked out Sept., 1973)

Card 16. Multicolor Plots (A10)

1-9 CHANGEPEN

**DEFAULT--no block marks on CALCOMP tape between treatment of ATOMRANGE cards.

PRØCK

Brookhaven Crystallographic Computer Program Writeup

Files: 9

PRØCK(INPUT,ØUTPUT,TAPE1,TAPE2,TAPE11,TAPE12,TAPE13,TAPE14,PUNCH)

Purpose:

Preliminary processing of single crystal diffraction data from automatic data acquisition programs at HFBR. Produces punched card and/or plot and/or tape output suitable for use in BNLABS or ABSØR, the programs used to calculate absorption corrections. There are several different options (see appendices) for determining which part of the profile is the peak.

Job statistics: Field length = 60 K_8, time, -about 2 sec/reflection if plotting is done otherwise about 15 reflections/second.

Files required:

TAPE1	Input from ØRACLE or EXAMØR
TAPE2	Output for input to BNLABS, ABSØR or CØRDAT. Optional.
TAPE11	Plot file. Optional
TAPE12	Profile listing file. Optional.
TAPE14	Special profile listing file. Optional.
INPUT	
ØUTPUT	
PUNCH	Optional.

Input data:

Card 1 Title card FØRMAT(1X,A9,7A10) Any information in cols 2-80.

Card 2 Control integers FØRMAT(9I5,F5.0,6I5). Control integers for program options as follows. (ICN(I), I = 1,9), BETTY1, (ICN(I), I = 11,16)

cols 1-5	ICN(1)	Number of tape files to be processed. Does not include any skipped files.
cols 6-10	ICN(2)	Number of records to be skipped in first file processed.
cols 11-15	ICN(3)	Number of files on input tape to be skipped before processing begins.
cols 16-20	ICN(4)	Number of records to be processed. Does not include number skipped (check ICN(7)!!!).
cols 21-25	ICN(5)	= 0 for new output tape. Supply TAPE2. = -1 for no output tape.
cols 26-30	ICN(6)	= maximum number of smoothed background points for which a background trend is allowed. (See appendix A).
cols 31-35	ICN(7)	= 0 if number in columns 16-20 controls processing. = -1 if processing to continue until end-of-file on last file for which processing is requested.

cols 36-40 ICN(8) = 0 for no plot.

= 1 if tape is to be written for CALCØMP plot. Supply TAPE11.

= -1 for fast plot omitting individual symbols and scales (see Plot output). Supply TAPE11.

cols 41-45 ICN(9) This integer together with ICN(11) and ICN(12) control the method of peak integration. Let IMID be the central point of the scan. Let IMAX be the position of the maximum count. Then

0 implies that the points from IMID - ICN(11) to IMID + ICN(12) are taken as belonging to the peak. All other points are taken to be background.

1 The data are smoothed to the highest degree and integration is carried out as described in appendix A.

2,3,4,5 moderate degrees of smoothing.

6 The smallest amount of smoothing available in the program is applied.

7 Background is taken as the ICN(11) points at the beginning of the scan and the ICN(12) points at the end of the scan. (Note that the data collection routines have the beginning of the scan at high 2θ, the end at low 2θ.)

8 The points from IMAX - ICN(11) to IMAX + ICN(12) are taken as belonging to the peak. All other points are background.

11,12,13,14,15,16 The data are smoothed corresponding to 1,2,3,4,5,6, but the smoothed profile is only used to determine the position of the peak. For integration real points are used.

99 The position of peak is determined in such a way that the relative error $\sigma(I)/I$ is "minimized" (appendix B). Real points are used for integration.

cols 46-50 BETTY1 = Scale factor, F or E format, do not use zero, useful to avoid truncation error with large monitor counts.

cols 51-55 ICN(11) = high angle increment. (See ICN(9).)

cols 56-60 ICN(12) = low angle increment. (See ICN(9).)

If the data are smoothed (ICN(9) = 1,2,3,4,5,6,11,12, 13,14,15,16) then ICN(11) and ICN(12) determine the range from the midpoint of the scan in which a maximum is sought. If there is none in this range, the peak will not be integrated, and a diagnostic will be printed out.

For $\sigma(I)/I$ minimization (ICN(9) = 99), ICN(11) is the number of background points (BETA in appendix B) used in the method. ICN(11) must be less than the actual number of points in one background. For reasonable data: ICN(11)=10% of the number of profile points. If ICN(12) is equal to 1 a tape is written with complete scan information for the reflections which were specially treated (see appendix B). In this case supply TAPE14. ICN(12)=0 if no special tape list required.

cols 61-65 ICN(13) = 0 if new TAPE12 written with scan information and its interpretation from the first pass.

= -1 no scan data written to TAPE12.

cols 66-70 ICN(14) = 0 for no punched output.

= 1 for punched output (on-line).

cols 71-75 ICN(15) = 0 if no reflections are to be rejected.

= 1 if the REJT routine is called to reject reflections.

cols 76-80 ICN(16) = fraction in 0.01 of σ by which smoothed points may differ to consider that peak is down to background for the smoothing options only.

Card 3. Attenuator scale factors. FØRMAT(6F10.2,I10)

cols 1-10 New attenuator scale factor 1.

cols 11-20 Old attenuator scale factor 1.

cols 21-30 New attenuator scale factor 2.

cols 31-40 Old attenuator scale factor 2.

cols 41-50 New attenuator scale factor 3.

cols 51-60 Old attenuator scale factor 3.

cols 61-70 IXXY = 0 if counts are to be scaled multiplying by the step size (in hundredths) and dividing by the monitor count (in thousands).
IXXY = 1 if step size and monitor not included in scaling.
IXXY = -1 if step size included but monitor not included in scaling.

(The attenuator scale factors are normally read from the data tape and are the "old values". These may be replaced by new values at this stage. If there is no change, punch both the new and old. If left blank, the output data tapes will not contain information on which scale factor was used. Attenuators may be used on the x-ray machine only. This card may be blank for neutron data.)

Card 4. FØRMAT(2I5,2F10.7,6F8.0)

cols 1-5 LØNG = 0 implies that standard 80 col card images are produced on TAPE2 as described below under Output data.

> 0 instructs the program to output the true sequence number with each reflection. This implies long output records of 90 columns.

cols 5-10 ITECH = 0 for x-ray data.
= 1 for neutron data.

cols 11-20 FLAMB = wavelength of radiation in Å.

cols 21-30	FACT	A number used in integration by the smoothing algorithm (ICN(9) = 1,2,3,4,5,6,11,12,13,14,15,16). Useful on split peaks. Program does not consider background to be reached unless the point has a count less than FACT times the maximum count. FACT is normally 1.0, and any point less than maximum is legitimate for background. Should not be too small or peaks with low peak-to-background ratios will not be properly integrated.

The following quantities are applied to produce output which has true values of the angles on TAPE2. Note, however, that no correction is made in the case of 2θ.

			SATT	MAIN	PICKER	
cols 31-38	PARTØ.	Parity of ω	-1	-1	-1	
cols 39-46	PARTP.	Parity of ϕ	+1	-1	-1	For PRØCK purposes only
cols 47-54	PARTX.	Parity of χ	+1	-1	-1	
cols 55-62	ØMZER.	ω_0	ω_0	ω_0	ω_0	See the BNLABS and ABSØR writeups.
cols 63-70	PHIZER.	ϕ_0	ϕ_0	ϕ_0	ϕ_0	
cols 71-78	CHIZER.	χ_0	$180+\chi_0$	χ_0	χ_0	

Card 5. FØRMAT(6F9.6) Reciprocal cell constants a^*, b^*, c^*, $\cos\alpha^*$, $\cos\beta^*$, $\cos\gamma^*$

Supply the following cards only if REJT Routine supplied with program is called.

Cards 6. FØRMAT(3I3,2I6) H,K,L,2θx100, sequence number for all reflections to be rejected. These values must be in the same order as occurring on input TAPE1. Note that any one rejection card only affects the first input record with matching parameters. If 2θx100 (or sequence number) is zero or blank, then the corresponding quantity or quantities are not checked.

Output data:

TAPE2(IØUT): one record per reflection
FØRMAT(3I3,2F10.1,F6.3,3F7.2,2I3,F8.2,F8.3,I2) if LØNG = 0 or
FØRMAT(3I3,2F10.1,F10.3,3F7.2,2I3,F8.2,F8.3,I2,I6) if LØNG > 0.

H,K,L	the indices of the reflection
ØBSI	the integrated intensity in the peak (including background)
BACK	the background intensity.
GEECØ	the scale factor that was used. Attenuator scale *BETTY1*Step Size/Monitor counts
ØM	the ω value at which the data was collected.
FI	the ϕ value at which the data was collected.
CHI	the χ value at which the data was collected.
ISL	the number of points included in ØBSI.
ISB	the number of points included in BACK.
ØBSF1	corrected number of counts in peak for use in calculation of statistical error.

BACFK corrected number of counts in background for use in calculation of statistical error.

IDENT = 0 for reflections with no attenuator.
= 1 for reflections with one attenuator.
= 2 for reflections with two attenuators.
= 3 for reflections with three attenuators.

(Note that IDENT = 0 unless attenuator scale factor card has been properly punched as noted above.)

INDEX = the sequence number for this reflection as supplied on TAPE1 (only if LØNG > 0).

TAPE2 is terminated by an EØF.

PUNCH: one card per reflection, same FØRMAT as TAPE2. Note PUNCH will use 80-column format, even if long 90-column records have been written on TAPE2.

TAPE11: May be submitted to CALCØMP for plot (if requested).

TAPE12: Will be a BCD tape (if requested) which may be separately listed to get peak profiles.

TAPE14: A BCD tape, which may be separately listed to get profiles of reflections which were specially processed. ("COMING AGAIN LATER" reflections)

ØUTPUT: H,K,L,ØBSI,BACK,ISIGNL,IBKGRN,B1,NP,B2,ATSCL,IPHI,IØHM, ITWØTH,ICHI,INDEX,IRECCT,IFILE,RECA(9),RECA(10).

where the quantities not defined above are:

ISIGNL = total intensity from approximate integration on-line.
IBKGRN = background under peak from approximate integration on-line.
B1 = number of points in first background.
NP = number of points in peak.
B2 = number of points in second background.
ATSCL = attenuator scale factor used.
IPHI,IØHM,ITWØTH,ICHI = 100. x setting angles as corrected for parity (except in the case of 2θ) and zero.
INDEX = sequence number of reflection on input TAPE1.
IRECCT = record number
IFILE = file number
RECA(9 and 10) are label from input TAPE1.

A table is given which contains full widths and half widths for the profile as a function of $\sin\theta/\lambda$ and $I/\sigma(I)$. The deviations of the peak centers (based on the half width) from the centers of the scan interval are given.

<u>Plot output:</u> one frame per reflection.

INDEX, H, K, L are printed.

Count vs. angle is plotted with the following characters at the positions of the raw data points (characters and scales are omitted if fast plots are selected).

P if point was used in peak
B if point was used in background
N if point was not used but was within range of center
D if point was otherwise not used.

A smoothed curve without points is also drawn, if the smoothing routines were used.

Replaceable Subroutine NREJT

After each reflection is read, the subroutine NREJT is called if so requested on control card.

SUBRØUTINE NREJT(H,K,L,ITWØTH,NREJ)

This subroutine should return with NREJ=1 if reflection is to be rejected. Otherwise NREJ=0. The subroutine supplied requires data cards 6 as discussed above.

Data Input from TAPE1.

The data to be processed is read from a coded tape usually available as output from the routine ØRACLE which is used to decollate the pool tapes. ØRACLE output may first be run through the checking program EXAMØR, which catches bad records with spurious data which could cause PRØCK to fail. TAPE1 must consist of 230 word binary records.
The following data words in the record RECA(230) are of consequence for PRØCK.

11, 12, 13, H, K, L in integer format

14, step scan size in 0.01 degrees

15, the time spent on each step

16, the number of background points in rough integration

17, the scan range in 0.01 degrees

18, the attenuator scale factor x 1000

19, the number of points in the scan

20, the total intensity by rough integration

21, the background intensity by rough integration

22, 23, 24, 25, ϕ, ω, 2θ, χ (x 100)

28, INDEX, the serial number of the observation assigned by the data collection routines

29, first point in scan

226, last allowed point in scan

Rest of record is blank or irrelevant

Appendix A: Smoothing and integration algorithm.

The raw data may be smoothed by a method described in Whitaker and Robinson ("The Calculus of Observations"). The degree of smoothing is a variable which should be selected so that narrow peaks with considerable intensity do not dip below the origin when smoothed, i.e., they should not look too much like sinx/x.

A peak (relative maximum) is sought within a specified distance of the scan center. Starting down from this peak in each direction, the points are considered as belonging to the reflection until the first difference between two successive points either changes sign (if ICN(16) = 0) or is less than ICN(16) times the standard deviation of the difference between the two points.

Background is now followed toward end-of-scan range until a trend is exhibited. A trend is defined as two or more successive first differences with the same sign. The number of such differences with the same sign allowed is an input parameter ICN(6).

The two backgrounds are added but are not subtracted from the total at this stage of the game.

Because of the smoothing, the variance of each of the smoothed points is not equal to the number of counts but is always less than this. For one point, the variance may be 0.35 times the number in the smoothed count, for two points it may be 0.50. These numbers are printed out as the "variance multipliers" at the beginning of the program. For each reflection, the variance of the total count and the variance of the background count are printed out as ØBSFI and BACFK. The variance of the final net intensity (calculated in the successor programs BNLABS or ABSØR) is then

$$\text{ØBSFI} + (\text{ISL}/\text{ISB})^2 * \text{BACFK}.$$

Appendix B: Peak position for "minimal" σ(I)/I" algorithm.

Ref. Lehmann and Larsen, Acta Cryst. A30, 580 (1974).

The points in the profile are called CØUNT(X). The profile is divided into two halves, the point of division being that of maximum counts, CØUNT(MAX). Look at the right-hand part. For this a function of J, σ(I(J))/I(J), is calculated. This function is based on the following points: CØUNT(MAX) .... CØUNT(J) .... CØUNT(J+BETA). The J-MAX+1 points CØUNT(MAX)...CØUNT(J) represent the peak, and their sum is P. The BETA points CØUNT(J+1)....CØUNT(J+BETA) represent the background, and their sum is B. BETA is a fixed number chosen by experience, but it must be less than the actual number of background points to guarantee some success. Now the function is

$$\sigma(I(J))/I(J) = \sqrt{P+(J-MAX+1)^2/BETA^2*B/(P-(J-MAX+1)/BETA*B)}$$

This function can be calculated for J=MAX ..... N-BETA, where N is the total number of points in the profile. The J giving a minimum for the function will be taken as the last point of the peak when moving from MAX.

A similar calculation is carried out for the left part of the profile. These two points determine the position of the peak.

Finally, BETA points are added to the width of the peak on each side, because in practice the algorithm comes up with peaks which are slightly too narrow.

In some cases a diagnostic: **coming again later** will be printed. This will happen in the following cases:

1) If no real minimum is found, i.e., if the minimum is J = N-BETA (or J = BETA+1).

2) If more than BETA/2 negative σ(I(J))/I(J) are observed. This means normally that the peak is very small.

3) If the difference between the two background averages is bigger than 3 sigma.

The program will redo these reflections and this calculation will supersede the previous one for output on TAPE2 (or cards).

In Case 1 the program will check the two backgrounds, and if they don't differ more than 3 sigma the original calculation is assumed to be good enough. Otherwise the program will try either to remove some of the background points or to incorporate some of the background in the peak.

In Case 2 a "peak" is placed in the center of the scan range. The width of this peak will be the one observed for other peaks in the same $\sin\theta/\lambda$ range.

In Case 3 the program will try to either remove some of the background points or to incorporate some of the background in the peak.

The intensity and the variance are in all cases calculated in the usual way, exactly as for ICN(9)=0. If ICN(12)=1 (and if TAPE14 is supplied), a special list of the reflections reexamined in the second pass will be given.

NB: One should always look at the plots or lists to ascertain that the integration has been done in a sensible way.

Normally, IXXY = 0, and the counts obtained for each step of the scan are normalized to account for experimental factors by multiplying them by the factor (2θ step size in 100ths of a degree)/(Monitor counts in 1000's). Usually the numerator will be in the range 6-14 and the denominator in the range 1-200. This factor is output on TAPE2 after multiplication by the scale factor supplied by the user on card 2.

NAME: PRØIN

AUTHORS: E. Meyer
T. Koetzle

CØRE: 50K (SCØPE 3.4)

TIME: approx. 40 secs for protein with 330 residues

DATE: February 1975

```
PRØGRAM PRØIN(TAPE10,TAPE11,INPUT,ØUTPUT,TAPE1,TAPE2,
              TAPE3,TAPE5=INPUT,TAPE6=ØUTPUT)
```

I PURPOSE: Prepares data for Protein Data Bank

II TAPES:

- TAPE1 - Scratch
- TAPE2 - Scratch
- TAPE3 - Raw data
- TAPE10 - Edited data
- TAPE11 - Error messages

III LIMITATIONS: none

IV REPLACEABLE SUBRØUTINES:

	ARGUMENT
A. IMP	NONE

V DECK SET UP:

A. JØB CARD

```
use SCØPE 3.4
MT1
default values for other parameters
```

B. CØNTROL CARDS

```
                                C219.
REQUEST,ØLDPL,E,HI,VSN=C493.                  get raw data PL
                                C495.
ATTACH,BUPD140,BUPD140,ID=CPRØGS.
BUPD140,Q,D,8,C=TAPE3.
REWIND,ØLDPL.
RETURN,ØLDPL.
ATTACH,PRØIN,PRØIN,ID=PDB.
REQUEST,TAPE10,*PF.
FTN,L,R=3,X,ØPT=2,PL=20000,A,SYSEDIT.         use only if supplying new
                                              IMP routine
LØAD,LGØ.
PRØIN.
REWIND,TAPE10,TAPE11.
CATALØG,TAPE10,EDITED DATA,ID=MYID,XR=MYID.   save edited data
REWIND,TAPE10.
CØPYSBF,TAPE10,ØUTPUT.                        print listing of edited data
CØPYSBF,TAPE11,ØUTPUT.                        print listing of error messages
```

BROOKHAVEN CRYSTALLOGRAPHIC COMPUTER PROGRAM

PRØGRAM PRØIN(TAPE10,TAPE11,INPUT,ØUTPUT,TAPE1,TAPE2,
TAPE3,TAPE5=INPUT,TAPE6=ØUTPUT)

PRØIN reads raw protein crystallographic data and edits these data into the standard Protein Data Bank format. This standard format is described in the writeup "Protein Data Bank-File Record Formats (September 1972)".

Files:	TAPE1	Scratch (may be used by SUBRØUTINE IMP)
	TAPE2	Scratch (used by SUBRØUTINE INPUT)
	TAPE3	Raw Data
	TAPE10	Processed Data in Standard FØRMAT (*DECK and *CWEØR,17 records at front)
	TAPE11	Error Messages

PRØIN uses SUBRØUTINE IMP to read raw data from TAPE3. The standard routine supplied will read data using a variable FØRMAT specification supplied at run time, and is suitable for data with the N atom occurring first in each residue and with the amino acid name on the same line as N. For data in a different form, a special IMP routine must be supplied.

Input:

The following information is read from the job's INPUT file.

1. Title Card FØRMAT(12A1,2A4,6A10)

Cols	1-12	Space Group Symbol (e.g. P 21 21 21) left justified (include blanks as indicated)
Cols	13-20	8-character identification code
Cols	21-80	Name of protein

2. Author Card FØRMAT(6A10)

Cols	1-60	Names of contributor and co-authors

3. Cell Card FØRMAT(6F9.6,I6,2I5)

Cols	1-9	a	Ångstroms
Cols	10-18	b	
Cols	19-27	c	
Cols	28-36	α	degrees
Cols	37-45	β	
Cols	46-54	γ	

7

Cols	55-60	Z	molecules per unit cell
Cols	61-65	ICN1	= 0 ØRIGX matrix read in ≠ 0 inverse ØRIGX matrix read in
Cols	66-70	ICN2	= 0 use standard SCALE matrix determined from cell constants = 1 read in SCALE matrix = 2 SCALE assumed identical to ØRIGX and submitted orthogonal coordinates are used as is.
Cols	70-75	ISKIP	cards to skip on TAPE3.
Cols	76-80	ICALF	= 0 for input of a full set of coordinates = 1 for input of C^{α} coordinates only.

4. ØRIGX Cards FØRMAT(4F10.5)

Cols	1-10	O_{11}
Cols	11-20	O_{12}
Cols	21-30	O_{13}
Cols	31-40	T_1

and so forth (3 cards total) punch zero fields as 0.0--do not leave blank.

5. SCALE Cards FØRMAT(4F10.5) Present only if ICN2=1.

Cols	1-10	S_{11}
Cols	11-20	S_{12}
Cols	21-30	S_{13}
Cols	31-40	TS_1

and so forth (3 cards total) punch zero fields as 0.0--do not leave blank.

6. FØRMAT CARD FØRMAT(8A10)

FØRMAT of data on TAPE3. If a blank card is used, the default Diamond FØRMAT(4F10.5,2I5,5X,F9.4,1X,A3,1X,I3,1X,7A1,2F6.2) is assumed. This card is read into the array FØRMT.

7. Remark Cards FØRMAT(6A10) optional (as many cards as desired). Do not punch beyond column 60.

8. Footnote Cards FØRMAT(6A10,I10) optional

Cols	1-60	Text
Cols	61-70	Footnote number

As many cards as desired. Footnotes are distinguished from remarks by having an integer in columns 61-70.

9. EØF

SUBRØUTINE IMP

The routine supplied reads from TAPE3 in the following order:

ATIVE(1)≡X_o ATIVE(2)≡Y_o ATIVE(3)≡Z_o	submitted coordinates
AANG	torsion angle (degrees)
IDW	atom type (this number is redefined by PRØIN to agree with the order of atoms on the DECØDE card, (generated internally), but is passed along for torsion angles)
NØ	sequence number (set equal to residue number by PRØIN if not supplied)
ECT	electron count
AA	amino acid name (should appear only once per residue opposite N atom)
NØSEQ	residue number
TAU(1)-TAU(2)	blank except for torsion angle records
TØM(1)-TØM(5)	five-character IUPAC atom name, one character per word, left justified
ØCC	occupancy
BEE	temperature factor

IMP must contain two labelled COMMON statements as follows:

```
CØMMØN/ZMAT/SCALE(3,3),A(3,3),B(3),FØRMT(8),Ø(3,3),T(3),S(3),ISKIP
CØMMØN/SPASS/W(3),AANG,IDW,NØ,LINØ,ECT,AA,NØSEQ,TAU(2),
TØM(5),ZIPFEL,ACTIVE(3),NØTE,NEND,IDLE,BEE,ØCC
```

FØRMT contains the FØRMAT of the data on TAPE3.

In addition to the data normally read from TAPE3 as indicated above, the following quantities in SPASS must be defined by IMP and returned to the main program:

LINØ	$1 \leq$ LINØ $\leq$ N line count (increment for each datum read and accepted from TAPE3
ZIPFEL	the first two characters in TØM--set with statements ENCØDE(2,5,ZIPFEL)TØM(1),TØM(2) 5 FØRMAT(2A1)
NØTE	footnote number (set equal to 0 if no footnote is present referring to atom in question)
IDLE	normally set equal to 0.
NEND	normally set equal to 0 with a DATA statement return with NEND=1 on data termination

Note: AANG should be set equal to 0.0 for atomic coordinate records (the standard IMP routine does this, and sets IDLE and NØTE to zero, as well).

The standard IMP routine supplied with PRØIN will reject atoms labelled 'DUMMY', or having 'D' in TOM(5). Atoms labelled 'CØ' are renamed 'C'. Several common errors in amino acid naming are also corrected: 'PRO' becomes 'PRØ', 'TRY' becomes 'TRP', and 'CYH' is changed to 'CYX'. In the case of 'TRY' the non-standard atom names which usually go with this designator are changed to the correct IUPAC names. IMP will accept Diamond Real Space output with no editing, and will skip bad records with illegal data. The contents of these bad records are listed on the output file and on TAPE11.

An ambiguity occurs because CYS is used for the name of both cysteine and cystine. The procedure adapted here is to employ CYX for cysteine (PRØIN then knows the residue is cysteine and computes the 9-digit ID number correctly; the name is internally set back to CYS). CYS is retained for cystine (disulfide bond).

PRØIN scans atomic symbols first as single character names and then, if no match is found, as double character names. This may lead to errors (e.g. Fe-Iron is identified as F-fluorine). The easiest way past this is to give an atom like Fe another single-letter name which is not in use, like V-vanadium, so it will be identified uniquely, and then edit later. The Fe-V switch has been implimented automatically, but other problem atoms, like Ca-calcium, will have to be edited by hand.

Error messages (on TAPE11)

In addition to a printout of bad records with illegal data in field, there are two types of error messages:

NØ AA indicating the amino acid name could not be recognized by PRØIN.

NØ ATNØ indicating the atom name could not be recognized.

In each case, PRØIN will write out the amino acid name, fractional coordinates, atom type number, sequence number, atom name, and line number.

TAPE11 also will contain a message giving the number of atoms read trom TAPE3 and accepted, and a list of bad records encountered on TAPE3.

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
*                                                                     *
****        BROOKHAVEN NATIONAL LABORATORY                            *
****        CHEMISTRY DEPARTMENT                                      *
*                                                                     *
****        CRYSNET UTITLITY PROGRAM                                  *
*                                                                     *
** NAME -- RMCOPY  - USER JOB                                         *
*                                                                     *
** AUTHORSHIP -- CONROL DATA CORPORATION AS 7000 COPY UTITLITIES      *
*           ADAPTED TO RMCOPY BY H.J. BERNSTEIN, BNL, 15-FEB-75.     *
*           SOFTWARE DEVELOPED UNDER CONTRACT AG-370 WITH THE NSF    *
*           UNDER THE AUSPICES OF ERDA.                              *
*                                                                     *
** ENTRY POINT -- RMCOPY                                              *
*                                                                     *
** PURPOSE -- TO COPY DATA FROM ONE FILE TO ANOTHER                   *
*                                                                     *
** CALLING SEQUENCE -- EXECUTED VIA CONTROL CARD. THE JOB ADVANCER    *
*           CRACKS THE PARAMETERS AND PLACES THEM STARTING AT THE    *
*           USERS  RAS+2.                                            *
*                                                                     *
** INPUT -- CONTROL CARD FORMAT IS                                    *
*                 -    -                  ENTRY POINT COPIES          *
*                 .    .                  TO EOI                      *
*                 . P  .                  N PARTITIONS                *
*                 . BF .                  ..                          *
*         RMCOPY,. CF .(LFN1,LFN2,N)      ..                          *
*                 . S  .                  N SECTIONS                  *
*                 . BR .                  ..                          *
*                 . CR .                  ..                          *
*                 . R  .                  N RECORDS                   *
*                 -    -                                              *
*                                                                     *
*           LFN1  IS THE ORIGINAL FILE  (DEFAULT = INPUT)             *
*           LFN2  IS OUTPUT FILE        (DEFAULT = OUTPUT)            *
*           N  IS THE NUMBER OF UNITS TO COPY.                        *
*                                                                     *
*           THE ARGUMENTS MAY BE REPEATED IN SETS OF FOUR, E.G.       *
*                 RMCOPY,BR,F1,NULL,3,BF,F1,F2.                       *
*                                                                     *
```

```
** OUTPUT -- THE INPUT FILE IS COPIED TO THE OUTPUT FILE, USING THE    *
*          DATA MANAGER, FROM THE CURRENT POSITION THROUGH THE         *
*          SPECIFIED NUMBER OF UNITS OR TO THE NEXT FILE DELIMITER     *
*          HIGHER THAN THE UNITS BEING COPIED.  FOR EXAMPLE,           *
*                 RMCOPY,S(IN,OUT,5)  WOULD COPY 5 SECTIONS FROM       *
*          IN TO OUT OR STOP AT EOP/EOI  IF ENCOUNTERED PRIOR TO       *
           5 SECTIONS.                                                 *
                                                                       *
*          DAYFILE MESSAGES --                                         *
*          ERROR                                                       *
*          *  UT000 - ILLEGAL PARAMETER*                               *
*          A PARAMETER WAS SPECIFIED ON THE CONTROL STATEMENT          *
*          LONGER THAN 7 CHARACTERS.                                   *
*          *  UT001 - INVALID NUMERIC DIGIT*                           *
*          A NON-NUMERIC DIGIT WAS FOUND IN N PARAMETER.               *
*          *  UT020 - RT=U MUST HAVE BT=K,RB=1*                        *
*          UNDEFINED FORMAT FILES MUST BE DESCRIBED BY A PRIOR         *
*          FILE CARD AS BT=K, RB=1.                                    *
*          *  UT021 - UNIDENTIFIED DATA EXIT TAKEN*                    *
*          THE DX WAS EXECUTED FOR OTHER THAN  EOI/P/S                 *
*          *  UT023 - COPY TERMINATED*                                 *
*          COPY ENDED FOR REASONS OTHER THAN HAVING COMPLETED          *
*          SPECIFIED DATA TRANSFER (N≠1) OR ENCOUNTERING A HIGHER      *
*          FILE DELIMITER THAN UNIT COPIED.  (WOULD BE LOGGED FOR N=0) *
*          *  UT037 - ERROR WHILE COPYING --*                          *
*          DATA MANAGER ERROR ON INPUT OTHER THAN EXCESS DATA.  UT037  *
*          WILL BE FOLLOWED BY THE DM ERROR.                           *
*          *  UT205 - S RECORD TOO LARGE FOR MRL SPECIFIED*            *
*          DM142 ERROR SHOULD FOLLOW.                                  *
*          *  RMNNN - ERROR ON FILE NAMED XXXXXXX*                     *
*                                                                      *
           TERMINATION                                                 *
           *  UT030 - COPY COMPLETE*                                   *
*          N UNITS HAVE BEEN SUCCESSFULLY COPIED, AS SPECIFIED.        *
*          *  UT031 - EOI ENCOUNTERED*                                 *
*          *  UT032 - EOP ENCOUNTERED*                                 *
*          *  UT033 - EOS ENCOUNTERED*                                 *
*          COPYR/S/P HAS ENCOUNTERED EOS/EOP/EOI                       *
*          *  UT034 -RECORDS/SECTIONS/PARTITIONS -                     *
*                    L          M          N*                          *
*          L RECORDS READ, M SECTIONS, N PARTITIONS.  IF NUMBER IS     *
*          ZERO, UNIT IS NOT INCLUDED IN THE MESSAGE.  MINIMUM IS 0 EOR*
*                                                                      *
*          WARNING                                                     *
*          *  UT200 - DATA IS LEFT-JUSTIFIED, ZERO FILLED*             *
*          IF INPUT (VARIABLE) MRL ≤ OUTPUT (F FORMAT) FL,             *
*          EXPLANATORY MESSAGE IS LOGGED.                              *
*          *  UT201 - EXCESS DATA WILL BE TRUNCATED*                   *
*          IF INPUT(VARIABLE) MRL ≥ OUTPUT (F FORMAT) FL, A WARNING    *
*          MESSAGE IS LOGGED.                                          *
*          *  UT202 - F/R/Z DATA TRUNCATED*                            *
*          AN EXCESS DATA ERROR OCCURRED ON AN F/R/Z INPUT FILE.       *
*          FULL GETS ARE NEEDED FOR A COMPLETELY COPIED RECORD.        *
*          TO ELIMINATE MESSAGE, CHECK INPUT MRL FOR ACCURACY AND      *
*          RAISE  FLS BEFORE THE COPY TO MORE THAN PREVIOUS RUN.       *
           *  UT203 - FILE IS NOT SEQUENTIAL*                          *
           INPUT OR OUTPUT FO IS NOT SEQUENTIAL.  THIS REMINDER IS     *
*          ISSUED BY THE SEQUENTIAL COPIES BECAUSE THE FILES ARE       *
*          TREATED IN AN ENTIRELY SEQUENTIAL MANNER, AND THE USER      *
*          IS RESPONSIBLE FOR DATA CONTINUITY.                         *
*          *  UT204 - LIBRARY COPY MAY BE LESS THAN ONE PARTITION*     *
*          COPYR OR COPYS WAS USED FOR COPYING A LIBRARY FILE, WHICH   *
*          IS ORGANIZED BY PARTITION.                                  *
```

```
*                                                                      *
** NOTE -- IN THE COPIES, AN ATTEMPT IS MADE TO USE FULL GETS          *
*         WHENEVER POSSIBLE, SO THE BUFFER IS ALLOCATED DYNAMICALLY.   *
*         IF MRL IS SPECIFIED, SCM ALLOCATED IS PROGRAM LENGTH PLUS    *
*         MRL, IF THE TOTAL IS .LE. CURRENT FLS OR A CONSTANT, MAXFL.  *
*         (CURRENTLY 30000).  IF MRL IS NOT SPECIFIED, MBL IS USED     *
*         INSTEAD.  IF  BOTH ARE ZERO, MAXFL IS ALLOCATED.             *
*                 FLS PRIOR TO THE COPY IS RESTORED AFTER.             *
*                                                                      *
*         ON NORMAL EXIT, ALL FILES ARE CLOSED.                        *
** EXIT -- NORMAL EXIT IS ENDRUN (USER PROGRAM)                        *
*         ERROR EXIT IS ABORT  OR  ABORT  LFN                          *
*                                                                      *
** REGISTERS SAVED -- COPY IS A USER PROGRAM                           *
*                                                                      *
** MACROS USED -- OPENM,MEMORY,GET,GETP,PUT,PUTP,FETCH,STORE,          *
*         MESSAGE,ENDRUN,ABORT,FILE,NXTCARD,WEOR,ENDFILE,SETFIT        *
*                                                                      *
** REGISTER USAGE --                                                   *
*          (OFTEN SAVED AND RESTORED FOR 6000 COMPAT)                  *
*                 A0 - UNIT DECREMENT FLAG (SET BY ENTRY-POINT)        *
*                 X4 - TRANSFER LENGTH DURING MOVE                     *
*         THE REST OF THE REGISTERS ARE GENERAL WORK REGISTERS         *
*                                                                      *
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
```

BNL CRYSTALLOGRAPHIC COMPUTER PROGRAM WRITEUP

SADIAN

PRØGRAM SADIAN(INPUT,ØUTPUT,TAPE6=ØUTPUT,TAPE5=INPUT)

SADIAN is a program which Searches for Atomic Distances and ANgles in crystal structures. It searches for all interatomic distances and/or bond angles within 26 unit cells surrounding the reference unit cell, up to specified limits. The program handles any symmetry from triclinic to cubic, and is written in FØRTRAN.

LIMITATIONS: 200 atoms, 48 symmetry operations, eight translations.

INPUT DATA

1) Title card (12A6). Columns 1-72 may contain any desired coded information.

2) Control Card (F10.7,5I3,F10.7,I3)

Columns

1-10 DMAX. Limit up to which distances are printed out (in Å). When DMAX = 0.0, calculation of atomic distances is bypassed, and no distance tables are printed.

11-13 NA. Number of atoms in asymmetric unit ($\leqslant$ 200).

14-16 NT. Number of translations ($\leqslant$ 8).
e.g., NT = 1 for P
NT = 2 for C or I
NT = 4 for F

17-19 NS. Number of symmetry positions ($\leqslant$ 48). For noncentric structures NS is equal to the number of equivalent points of the general position divided by NT. For centrosymmetric structures it is one-half this number.

20-22 ICENT = 1, if there is a symmetry center at the origin of the unit cell.

ICENT = 2, if there is none.

23-25 NW = 0, no bond angles will be calculated.

NW = -1, bond angles A-CA-B will be calculated around all atoms, when CA-A and CA-B, the sides of the angles are smaller than AMX.

NW > 0 is the total number of the angle control cards for the atoms around which bond angles will be calculated, in case one wishes to know the bond angles around selected atoms only (NW $\leqslant$ NA). (See Input 7).

26-35 AMX. Limit for the sides of the angles to be calculated (in Å). When AMX is given as a negative value, not only A-CA-B, but also the angles CA-A-B and CA-B-A will be computed.

36-38 IDR = 0 for direct cell constants, = 1 for reciprocal cell constants

3) Cell constant card (3F9.4,3F9.6)

Columns

1-9,10-18,19-27 a,b,c,cosα,cosβ,cosγ or

28-36,37-45-,46-54 a^*,b^*,c^*,cosα^*,cosβ^*,cosγ^*. The format is the same as in FLINUS and other programs.

4) Atomic parameter cards (A6, 21X, 3F9.6/) Not more than 200 Atoms

Columns

1-6 Atom identification (Hollerith)

7-27 Irrelevant

28-36,37-45,46-54 x_i, y_i, z_i fractional coordinates for atom i.

The format is the same as in FLINUS. The punch output of FLINUS may be used as input here . Each atom parameter must be followed by another card. Information on this second card is irrelevant. This allows use of parameter cards from FLINUS without removing temperature factor cards. -- x_i, y_i and z_i may have any value: they can be negative or greater than one.-- Before the program proper starts a subroutine is called by means of which the parameters of certain atoms can be set equal to each other in case of special positions. A dummy subroutine with a return statement is supplied with the deck:

```
SUBRØUTINE  SETXYZ(XYZ)
DIMENSIØN  XYZ (4, 200)
RETURN
END
```

Here XYZ(1,I) corresponds to the identifier of atom I, while XYZ(2,I), XYZ(3,I) and XYZ(4,I) correspond to x_i, y_i, z_i.

5) Translation cards (3F10.8). No more than 8 cards, but at least one.

Columns

1-10,11-20,21-30 T_x, T_y, T_z, translations in the x, y, z-directions, expressed as fractions of the cell edges and corresponding to the centering of non-primitive lattices. For primitive lattices a blank card must be submitted.

6) Symmetry cards (3(F15.9, 3F3.0)). Not more than 48 cards.

Columns

1-15,25-39,49-63 TTS_x, TTS_y, TTS_z. Translational parts of the expression for the equivalent position, in direction x, y, and z.

16-18,19-21,22-24 Multiplier (TS_x)1,2, and 3 of x, y and z for x'.

40-42,43-45,46-48 Multiplier (TS_y)1,2, and 3 of x, y and z for y'.

64-66,67-79,7-72 Multiplier (TS_z)1,2, and 3 of x, y and z for z'.

The format is the same as in FLINUS. -- The definition of x', y' and z' is:

$$x' = TTS_x + (TS_x)_1*x + (TS_x)_2*y + (TS_x)_3*z$$

$$y' = TTS_y + (TS_y)_1*x + (TS_y)_2*y + (TS_y)_3*z$$

$$z' = TTS_z + (TS_z)_1*x + (TS_z)_2*y + (TS_z)_3*z$$

7) Angle control cards (F6.3, 22I3), optional, necessary only when NW > 0.

Columns

1-6 AMAX, the same as AMX but it applies only to the atom, the number of which is given in column 7-9.

7-9 CA, number of the nth central atom, around which bond angles have to be computed. The numbering must be the same as in the sequence of the atomic parameter cards.

10-12 CN = 0, all bond angles around CA will be calculated where CA-A and CA-B are smaller than AMAX.
CN > 0, is the total number of coordinated atoms around CA, in case one wishes to select the bond angles, in which CA and the coordinated atoms enumerated in CØAT are involved (CN ≤ 20).

13-15,16-18,...,70-72
CØAT, numbers of the coordinated atoms. Again, as for CA, the numbers here are the consecutive numbers of the atoms in the list of atomic parameters.

OUTPUT:

1) Title
2) NA, NT, NS, ICENT
3) Cell constants
4) Atomic parameters, after having been set by the subroutine SETXY2
5) Translations
6) Symmetry positions
7) DMAX, AMX, NW
8) Angle control cards

9) Atomic distances:
   a) Identification of atom 1
   b) x, y, and z of atom 1
   c) Identification of atom 2
   d) x', y', and z' of atom 2
   e) Distance from atom 1 to atom 2 (in Å)
   f) Number of symmetry position, which has been used in computing x', y', and z' of atom 2.
   g) Number of translation, which has been used in evaluating x', y' and z' of atom 2.
   h) Number of the unit cell in which atom 2 is located.

10) Bond angles:
   a) Coordinates of CA
   b) Identification of the 3 atoms, A-CA-B, involved in the angle.
   c) Bond angle (in degrees)
   d) Coordinates of A
   e) Distance CA-A (in Å)
   f) Coordinates of B
   g) Distance CA-B (in Å)
   h) Distance A-B (in Å)
   i) Identification and bond angles of CA-A-B and CA-B-A

All atomic coordinates in d) range from 0.0 to 3.0, and refer to one common origin for all 27 considered unit cells. In unit cell 1, x' y' and z' are from 0.0 to 1.0, in cell 27 from 2.0 to 3.0. Atom 1 is always situated in cell 14, where x, y and z go from 1.0 to 2.0. In counting from cell 1 to cell 27 z changes most rapidly, x least rapidly. If ICENT = 1, the centrosymmetrically related atomic positions, which do not show up in the list of symmetry positions, are distinguished by having an asterisk behind the number of the unit cell.

NAME: SANDA AUTHOR: L. Andrews

CORE: 37K DATE: March 1974

PROGRAM SANDA(INPUT,ØUTPUT,TAPE3)

I. PURPOSE:

To calculate all distances and angles.

II. TAPES:

none

III. LIMITATIONS:

A. Symmetry-atoms Dimension-175

IV. REPLACEABLE SUBROUTINES:

none

V. DECK SET UP

A. JOB CARD

1. TIME LIMIT - 8 secs
2. FIELD LENGTH - 37K
3. NUMBER OF TAPES - 0
4. ECS - 0

B. CONTROL CARDS

```
ATTACH(SANDA,SANDA,ID=CPRØGS)
SANDA.
```

C. DATA CARDS:

CARD	FORMAT
1. Title card	20A4
2. Cell Constant card	7F7.3,3F7.4
3. Control card	3I4,2F6.2,I4,F6.2,2I4,3F4.0,2I4
4. Symmetry cards	F11.6,2I2,F11.6,2I2,F11.6,2I2

D. REMOTE FILES:

1. ØUTPUT: The atoms and their input coordinates are listed and each atom is assigned a serial number. The symmetry operations are also assigned serial numbers. The bonded atom pairs are then listed labelled by the serial numbers of the terminal atoms. The first atom of each pair is in its input position. The second atom has its correct coordinates listed and also which symmetry transformation was used; the ØRTEP convention is used to output which unit cell the second atom is in (with respect to its original position).

Brookhaven Crystallographic Computer Program

NAME: SANDA FILES: 3 TIME: 10 sec

CORE FL: 37K

PRØGRAM SANDA(INPUT,ØUTPUT,TAPE3)

DATA CARDS

Card 1 TITLE CARD (72H) - Any alpha-numeric information desired as a title line. This may be a blank card.

Card 2 CELL CONSTANT CARD (3F7.3, 3F7.4)

Column 1-7	8-14	15-21	22-28	29-35	36-42
a	b	c	cosα	cosβ	cosγ

These are the unit cell edges in Å and the cosines of the interaxial angles. If an angle is 90°, leave the corresponding field blank.

Card 3 CONTROL CARD (3I4,2F6.2,I4,F6.2,2I4,3F4.0,2I4)

Column	Content
1-4 (N)	Total number of coordinate cards (≤175)
5-8 (M)	Total number of symmetry cards (≤192) 2
12 (NCARD)	0 or Blank = Atomic positional parameter cards only used
	1 = Atomic positional and thermal parameter cards used
13-18 (DMAX)	Maximum distance to calculate Default = 1.7 Å
19-24 (DMIN)	Minimum distance to calculate Default = 0.0
28 (JAGL)	0 or Blank = Calculate distances only
	1 = Calculate both distances and angles
	2 = Calculate angles only
29-34 (DANG)	Maximum distance to be used in angle calculation
38 (ITRN)	0 or Blank = All translations
	1 = No translations
42 (ISOR)	0 or Blank = No sorting
	1 = Sort on distances
43-46 (TR)	Number of grid points in X direction } blank gives 1.0
47-50 (TS)	Number of grid points in Y direction } blank gives 1.0
51-54 (TT)	Number of grid points in Z direction } blank gives 1.0
58 (IS1)	0 = LINUS format atomic parameters
	1 = X-ray format
	2 = UCLALS format
62 (IS2)	1 = Grid coordinates
	2 = Decimal fractional coordinates

Card 4 SYMMETRY CARDS (F11.6,2I2,F11.6,2I2,F11.6,2I2)

One for each symmetry operation in the space group, the identity first. Refer to International Tables, Vol. I.

SYMMETRY	DIGIT
x	1
-x	-1
y	2
-y	-2
z	3
-z	-3

COLUMN	CONTENT
1-11	Translational part of x
12-13, 14-15	Symmetry for x direction
16-26	Translational part of y
27-28, 29-30	Symmetry for y direction
31-41	Translational part of z
42-43, 44-45	Symmetry for z direction

Card 5 ATOMIC PARAMETER CARDS

a) POSITIONAL b) THERMAL

One positional parameter card per atom is required. The total number must equal the number in cols. 1-4 of the Control Card. The program does not use the thermal parameter cards but, if they are supplied, a 1 must be punched in col. 12 of the Control Card.

ATOMIC POSITIONAL PARAMETER CARD

a) X-RAY 70 FORMAT (7X,A2,A4,3F8.4)

COLUMN	CONTENT
1-7	Blank
8-9	Atom Type (Left justify)
10-13	Type Identification (Right justify)
14-21	x coordinate in decimal fraction or grid points
22-29	y coordinate in decimal fraction or grid points
30-37	z coordinate in decimal fraction or grid points

b) LINUS FORMAT (A6,3X,5F9.6,2F6.2)

COLUMN	CONTENT
1-6	Atom Identifier (Any 6 Alpha-numeric characters)
7-9	Blank
10-27	Two numeric fields which are ignored
28-36	x coordinate in decimal fraction
37-45	y coordinate in decimal fraction
46-54	z coordinate in decimal fraction
55-66	Two numeric fields which are ignored

c) UCLALS FORMAT (5F10.5,I2,18X,A6)

COLUMN	CONTENT
1-10	x coordinate in decimal fraction
11-20	y coordinate in decimal fraction
21-30	z coordinate in decimal fraction
31-70	Not used
71-76	Atom Identifier (Any 6 Alpha-numeric characters)

N.B. If this program is to be used to calculate distances from atomic parameters produced from UCLALS refinement in mixed anisotropic-isotropic mode, the atomic parameter output will consist of two cards per anisotropic atom and one per isotropic atom. In this case, it will be necessary to either

1) remove the second card from the anisotropic atoms and use zero or blank in col. 12 of the control card or

2) insert blank cards after each isotropic atom and use 1 in col. 12 of the control card.

This is a possibility also from X-RAY 70 refinement procedures--so be cautious.

Brookhaven Crystallographic Computer Program

NAME: SCAT FILES: 3 TIME: 5 sec

CORE FL: 30K

Purpose: Produce X-ray scattering factor cards for FLINUS.

PROGRAM SCAT(INPUT,ØUTPUT,PUNCH,TAPE5=INPUT,TAPE6=ØUTPUT,TAPE7=PUNCH)

Input Data: Any number of cards of the following type

cols 1-4 atom type name from the list on the last page
Format (A4)

Output: Cards are produced for FLINUS until an EØF or unrecognized atom is found. A message is written on ØUTPUT when an unrecognized atom name is encountered.

Method: The program contains the coefficients distributed by Cromer for calculation of scattering factors by the method of Cromer and Mann.

$$SF(SINT) = C + \sum_{i=1}^{4} A_i * \exp(B_i * SINT*SINT)$$

where:

SF is a particular value of the scattering factor
SINT is sin theta over lambda
A_i, B_i, C are the coefficients given by Cromer

References:

D. T. Cromer and J. B. Mann, Acta Cryst. A24, 321-324 (1968).

D. T. Cromer and D. Liberman, J. Chem. Phys. 53(5), 1891-1898 (1970).

R. F. Stewart, E. R. Davidson and W. T. Simpson, J. Chem. Phys. 42(9), 3175-3187 (1965).

Common:

H	SDS	O-1	HF	CR	RHF	CO+2	RHF	BR	RHF
H AT	HF	F	RHF	CR+2	HF	CO+3	HF	BR-1	RHF
H-1	HF	F-1	HF	CR+3	HF	NI	RHF	I	RHF
LI	RHF	P	RHF	MN	RHF	NI+2	RHF	I-1	RHF
LI+1	RHF	S	RHF	MN+2	RHF	CU	RHF	W	RHF
B	RHF	CL	RHF	FE	RHF	CU+1	RHF	W+6	DS
C	RHF	CL-1	RHF	FE+2	RHF	CU+2	HF	HG	RHF
CVAL	HF	K	RHF	FE+3	RHF	ZN	RHF	HG+1	DS
N	RHF	K+1	RHF	CO	RHF	ZN+2	RHF	HG+2	DS
O	RHF								

Less Common:

HE	RHF	SE	RHF	IN+3	DS	TB+3	DS	PB	RHF
BE	RHF	KR	RHF	SN	RHF	DY	RHF	PB+2	DS
BE+2	RHF	RB	RHF	SN+2	RHF	DY+3	DS	PB+4	DS
NE	RHF	RB+1	RHF	SN+4	RHF	HO	RHF	BI	RHF
NA	RHF	SR	RHF	SB	RHF	HO+3	DS	BI+3	DS
NA+1	RHF	SR+2	RHF	SB+3	DS	ER	RHF	BI+5	DS
MG	RHF	Y	RHF	SB+5	DS	ER+3	DS	PO	RHF
MG+2	RHF	Y+3	DS	TE	RHF	TM	RHF	AT	RHF
AL	RHF	ZR	RHF	XE	RHF	TM+3	DS	RN	RHF
AL+3	HF	ZR+4	DS	CS	RHF	YB	RHF	FR	RHF
SI	RHF	NB	RHF	CS+1	RHF	YB+2	DS	RA	RHF
SI V	HF	NB+3	DS	BA	RHF	YB+3	DS	RA+2	DS
SI+4	HF	NB+5	DS	BA+2	DS	LU	RHF	AC	RHF
AR	RHF	MO	RHF	LA	RHF	LU+3	DS	AC+3	DS
CA	RHF	MO+3	DS	LA+3	DS	HF	RHF	TH	RHF
CA+2	RHF	MO+5	DS	CE	RHF	HF+4	DS	TH+4	DS
SC	RHF	MO+6	DS	CE+3	DS	TA	RHF	PA	RHF
SC+3	HF	TC	RHF	CE+4	DS	TA+5	DS	U	RHF
TI	RHF	RU	RHF	PR	RHF	RE	RHF	U+3	DS
TI+2	HF	RU+3	DS	PR+3	DS	OS	RHF	U+4	DS
TI+3	HF	RU+4	DS	PR+4	DS	OS+4	DS	U+6	DS
TI+4	HF	RH	RHF	ND	RHF	IR	RHF	NP	RHF
V	RHF	RH+3	DS	ND+3	DS	IR+3	DS	NP+3	DS
V+2	RHF	RH+4	DS	PM	RHF	IR+4	DS	NP+4	DS
V+3	HF	PD	RHF	PM+3	DS	PT	RHF	NP+6	DS
V+5	HF	PD+2	DS	SM	RHF	PT+2	DS	PU	RHF
MN+3	HF	PD+4	DS	SM+3	DS	PT+4	DS	PU+3	DS
MN+4	HF	AG	RHF	EU	RHF	AU	RHF	PU+4	DS
NI+3	HF	AG+1	DS	EU+2	DS	AU+1	DS	PU+6	DS
GA	RHF	AG+2	DS	EU+3	DS	AU+3	DS	AM	RHF
GA+3	HF	CD	RHF	GD	RHF	TL	RHF	CM	RHF
GE	RHF	CD+2	DS	GD+3	DS	TL+1	DS	BK	RHF
GE+4	HF	IN	RHF	TB	RHF	TL+3	DS	CF	RHF
AS	RHF								

Abbreviations:

HF	Hartree-Fock	RHF	relativistic HF
SDS	Stewart-Davidson-Simpson	AT	atomic
DS	Dirac-Slater	VAL	valence

NAME: SEARCH

CORE: SCM 70K
LCM $(16*NATØMS)_8$, where NATØMS = number of atoms in protein data set

PRØGRAM SEARCH(TAPE1,TAPE10,TAPE11,TAPE12,INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT)

I. PURPØSE:

To read a protein data set from the Protein Data Bank, extract a desired subset of atomic coordinates, and generate a connectivity table for display programs.

II. FILES:

TAPE1 - protein data set in standard Protein Data Bank format

TAPE10 - print file contains a listing of the atomic coordinates on TAPE1 along with detailed intermediate results

TAPE11 - display file with connecticity table

TAPE12 - X-ray system type atoms cards for input to PRJCTN

III. LIMITATIØNS:

For execution only on 7600 (SCØPE 2 or on large 6600 (SCØPE 3.4);
NATØMS $\leq$ 10,000;
Up to 1,000 atoms may be selected for display

IV. REPLACEABLE SUBRØUTINES:

none

V. DECK SET UP:

```
JØB,CP70,EC64,T77,YD1.
ACCØUNT(NAME,#)
MØUNT(VSN=CHEMØ1,SN=CHEM)
ATTACH(BUPD140,BUPD140,ID=CPRØGS,SN=CHEM)
ATTACH(ØLDPL,PDBPL,ID=PDB,SN=CHEM)
BUPD140(Q,D,8,C=TAPE1)
RETURN(ØLDPL)
ATTACH(SEARCH,SEARCH,ID=PDB,SN=CHEM)
FILE(TAPE12,RT=Z,BT=C,FL=80)
REQUEST(TAPE12,*PF)
SEARCH.
```

LCM sufficient for 2,000 atoms in protein file

```
CATALØG(TAPE12,SEARCHØUTPUTFØRPRJCTN,RP=100,ID=MYID,ST=MFA,AC=#)
REWIND(TAPE12)
CØPYSBF(TAPE12,ØUTPUT)
7/8/9
*C,DECKNAME          where Deckname is the deckname for the protein
                     of interest in the master update file.
7/8/9
        SEARCH data cards as described in writeup
6/7/8/9
```

Note: to retrieve the 6600 catalog file SEARCHØUTPUTFØRPRJCTN at the CRYSNET terminal, proceed as follows:

```
login under INTERCØM
ATTACH,XX,SEARCHØUTPUTFØRPRJCTN,ID=MYID
CØPYSBF,XX,TT
{ØFF,LP1}
{DEFINE,LP1,BANØFF}
ØN,LP1
"control" D
SEARØP
BATCH,TT,PRINT,MINE,HANS
WAIT FØR H,S display which signifies completion of transmission
"control" D
KB:     to close print file
logout
```

The SEARCH output file (TAPE12) should now reside on the PDP 11 disk as SEARØP under the user's UIC.

Brookhaven Crystallographic Computer Program

NAME: SEARCH FILES: 5 TIME: $<100_8$ secs.

CORE FL: $70K_8$

LCM FL: $(16*NATOMS)_8$

Purpose: To read a protein data set from the Protein Data Bank, extract a desired subset, and generate a connectivity table for display programs.

PRØGRAM SEARCH(TAPE1,TAPE10,TAPE11,TAPE12,INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT)

Method: Coordinates of points and radii are input sequentially following the protein data set. SEARCH orthogonalizes and scales to Angstroms the atomic coordinates. It then writes atoms within reach onto an extended core (ECØRE). If the number of atoms extracted exceeds a maximum (currently 1000), the radius is decreased, the atoms then within reach are counted, and this process is continued until the number of atoms is less than the working maximum. Then, a modification of UMZUG sets up the connectivity table. The total, extracted list is written on file TAPE11. TAPE12 contains the extracted list in x-ray system format for direct input into PRJCTN.

Internal Operation: SEARCH reads atomic coordinates and writes 8 words per atom into ECØRE

X(1), X(2), X(3), = fractional coord
X(4) = NATØ(NAT) atomic number
X(5) = atom name (coded)
X(6) = AA tags
X(7), X(8) = Encoded values of X(5), X(6)

Using various criteria,

SEARCH reads the above data from ECØRE and selects certain atoms: this list is added to the one above in ECØRE and consists of 8 words per atom:

W(1), W(2), W(3) = fractional coord
W(4), W(5), W(6) = orthogonal Å coord
W(7) = radius from pt.
W(8) = orig. atom input sequence number.

When the final radius is chosen,

UMZUG reads the ECØRE and stores the X,Y,Z (fract.), RX,RY,RZ (orthogonal), MUNCH (1 to max) = input seq. no., W(8).

Input:

One card for each SEARCH--FØRMAT(2I5,2F5.2,6A10)MANUS,NSHIFT,RADIUS,
RADMIN,M1,M2,M3,GTIT(3)

MANUS < -99 Terminator
< 0 extract all atoms in the range /MANUS/ ≤ atom type(DD) ≤ /NSHIFT/
Cols 1-5 0 SEARCH for all atoms within the radius of point: X,Y,Z (see below)
1 find the first atom in the list matching M1, then locate all atoms within the radius
2 for each atom matching M1, find all atoms within the radius
3 for each atom matching M1, find all atoms matching M2 and M3 within the radius

NSHIFT = 1 SEARCH asymmetric unit only
Cols 6-10 2 SEARCH symmetrically related atoms also
3 SEARCH symmetrically related atoms and apply translations to the 26 neighboring cells
11-15 RADIUS maximum radius
16-20 RADMIN minimum radius
22-30 M1 X (coordinates of origin point of SEARCH decoded
32-40 M2 or Y into 3F10.5 format)
42-50 M3 Z IF MANUS=0

M1, M2, M3 are 9-digit SEARCH codes in the form A/BBB/CC/DD/E as defined by PRØIN:

A = aqueous property
1 = hydrophobic
2 = hydrophyllic
3 = polar, -charge
4 = polar, +charge
5 = amide residue
6 = cyst (ei/i)ne
7 = glycine

B = amino acid sequence number
C = amino acid type (cf. dictionary)
D = numerical expression of the position of the atom of Appendix 2, Protein Data Bank File Record Format
E = atom type, according to the order of the Protein Data File

GTIT(3) is a 30 character title which is used as a header for files TAPE11,TAPE12. TAPE1 contains a protein file from the Protein Data Bank. This may be gotten from the data bank UPDATE tape.

Output:

The job's output file contains cell and symmetry information, selected atoms, connectivities, and a copy of TAPE1.

TAPE10: comments and error messages
TAPE11: selected atomic coordinates
Card 1. (5X,3A10) title
Card 2. (5I3,2X,5A10)

cols 1-5	IFRØM	number of atoms selected
cols 4-6	IRING	number of ring closures for connectivity
cols 7-9	NCENT	=1 for acentric =2 for centric
cols 10-12	NØRTH	not used
cols 13-15	NEQV	number of symmetry cards
cols 18-68	TITLE	from CØMPND card in data bank

Card 3. (6F9.3) ABC,ANG
cols 1-9 a
cols 10-18 b
cols 19-27 c
cols 28-36 α degrees
cols 37-45 β
cols 46-54 γ

Cards 4. (A10,17X,3F9.6,8X,A10) compatible with FLINUS
cols 1-10 DU(6) atom designation (amino acid name in cols 1-3; residue number in cols 4-6; CA, CB, etc in cols 7-10).
cols 28-36 X
cols 37-45 Y
cols 46-54 Z
cols 63-72 M (9 digit code)

Cards 5. (15I5)
connectivity "from" list IFRØM total entries

Cards 6. (15I5)
Ring closure list IRING total entries

Cards 7. (3(F15.0,3F3.0)) NEQV Symmetry cards
FLINUS format

Card 8. (I5)
cols 4-5 -0 terminator

TAPE12:
Card 1. (5X,3A10) Title
Card 2. CELL card
Cards 3. ATØM cards
Card 4. END card

Several examples of SEARCH procedures may be helpful:

Example 1. The active site contains His 57; extract all atoms within 10.0 Å of the epsilon 2 Nitrogen of His 57
M1 = 0/057/14/11/2
the input file would then contain one data card as follows:
1 1 10.0 005714112

Example 2. Find all charged groups within 7.0 Angstroms of one of the terminal N atoms in lysine in a protein known to have no cysteine.
M1 = 0/000/15/14/0
M2 = 0/000/00/00/2 Nitrogen atom
M3 = 0/000/00/00/3 Oxygen atoms
the data card would be
3 3 7.0 000015140 000000002 000000003
this will find all oxygen or nitrogen atoms within 7 Å of the terminal N atom of each lysine, with symmetry and translation operations added.

Example 3. Locate all O-N or O-O hydrogen bonds within a given molecule

M1 = 0/000/00/00/3 3 = oxygen
M2 = 0/000/00/00/3
M3 = 0/000/00/00/2 2 = nitrogen

the data card would be:

3 1 3.5 2.5 000000003 000000003 000000002

locates all oxygen atoms in the structure and then SEARCHES for all N or O atoms within 2.5 to 3.5 Å (assumed max. H bonding distance).

Example 4. Extract all backbone atoms of a protein.
(N.B. present maximum = 1000 atoms. If the protein has more than ∿250 amino acids, set NSHIFT=3.)

MANUS = -1, NSHIFT = 4, RADIUS = 999., RADMIN = 0.5

The data card would be

-1____4_999.__0.5___

The file is so organized that DD for CA = 1, amide N = 2, carboxyl C = 3, carbonyl O = 4.

Therefore if MANUS = -1 and NSHIFT = 3, one extracts only CA,N,C, the main backbone.

NAME: STRØNG
May - 1974
Author: Richard Love

Brookhaven Crystallographic Computer Program

NAME: STRØNG CORE: 26 K_8 TIME: < 30 SEC_8

PRØGRAM STRØNG(INPUT,ØUTPUT,TAPE5=INPUT,TAPE6=ØUTPUT)

I. Purpose:

A program to calculate strong neutron intensities from a known structure. STRØNG will list all unique reflections appropriate to the user's cell type which have an INTENSITY greater than 1.0. A separate list of reflections, within a specified 2θ range and sorted on intensity, is produced for use in conjunction with the RECF crystal orientation program ØRIENT.

II. Deck set-up:

A. JOB CARD

1. Time limit - 30 sec_8
2. Field length - 26 K_8
3. Number of tapes - 0
4. ECS - 0

B. CONTROL CARDS

```
ATTACH(STRØNG,STRØNG,ID=CPRØGS)
STRØNG.
```

C. DATA CARDS

1. Title card (8A10).

2. First parameter card (6I5).

   a) Centric or acentric. ICENT=1 or 0.
   b) Cell type, TRI=1, MØNØ=2, ØRTH=3, 4/MMM=4, 6/MMM=5, M3M=6.
   c) Number of symmetry elements, NS.
   d) Number of atomic coordinates, NA.
   e) Maximum number of reflections to be sorted and printed out as a separate list, INUM.
   f) Lattice type (P=0,C=1,I=2,F=3).

3. Second parameter card (4F10.6).

   a) Wavelength, LMDA.
   b) Minimum two theta for sorted list, TTMIN.
   c) Maximum two theta for sorted list, TTMAX.
   d) General temperature factor (to be added to the individual temperature factors), XXB.

4. Real unit cell parameters (6F9.6) (in Angstroms and degrees) A,B,C,ALPHA,BETA,GAMMA.

5. Symmetry transformations as defined in the FLINUS write-up (3(F15.4,3I3)). Note, for centric space groups (ICENT=1) do not include cards for positions related by a center of symmetry.

6. Atomic information list for one asymmetric unit (A9,5F9.6).

   a) Atomic identification.
   b) Neutron scattering length, XSF.
   c) Atomic multiplicity, XMULT.
   d) Atomic coordinates, XX,XY,XZ.

7. Individual (isotropic B) temperature factors, XB (F9.6).

<u>NOTE</u> Anisotropic temperature factors are not presently accommodated.

Cards 6 and 7 alternate for NA atoms. As in FLINUS, the overall temperature factor, XXB, is added to the individual temperature factors.

III. <u>Limitations</u>:

a) The array storage for atomic coordinates is set at 200. Thus, for centric structures, there can be no more than 200 atoms in a half unit cell; and for acentric structures there can be no more than 200 atoms in a full unit cell, i.e. the relation NA.NS $\leq$ 200 must hold. These parameters may be altered in common /AT/.

b) The array storage for the sorted array of reflections is limited to 251. Thus, the value of INUM cannot exceed 250. This parameter may be changed in array AR(3,251). The array size must be one larger than the maximum value of INUM.

OCTOBER, 1975

BROOKHAVEN CRYSTALLOGRAPHIC COMPUTER PROGRAM WRITEUP

TLS6

```
PROGRAM TLS6(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,PUNCH)

VERSION OF 30 MAY 1967

SJL MODIFICATION 2 : 22 JULY 1967
SUBROUTINE KAY CORRECTED BY T KOETZLE BNL 12-8-72
SO THAT IT NOW GIVES CORRECT XT IN L PRINCIPAL AXIS SYSTEM

 WRITEUP MODIFIED BY FLIEG HOLLANDER MAY 75 TO BEST OF HIS ABILITY

RIGID BODY MOTION ANALYSIS BY THE METHOD OF SCHOMAKER AND
TRUEBLOOD, INCLUDING THE SCREW TENSOR S.  THIS ANALYSIS WILL BE
PUBLISHED IN DETAIL IN ACTA CRYST., PROBABLY IN JAN. 1968.

INPUT B(IJ) ASSUMED TO HAVE INTRINSIC FACTOR OF 2, I.E., TEMPERA-
TURE FACTOR EXPONENT IS ASSUMED TO BE IN THE FORM
B11*(H**2)+B22*(K**2)+B33*(L**2)+B12*(H*K)*2+B23*(K*L)*2+B13*(H*L)
WHERE BIJ REPRESENT BETAS, B'S OR U'S

ALL CALCULATIONS REFERRED TO ORTHOGONAL AXIAL SYSTEM WITH FIRST
AXIS PARALLEL TO A, SECOND TO C*-CROSS-A AND THIRD TO C*.
MAXIMUM NUMBER OF ATOMS = 100.

  THIS PROGRAM INCLUDES PROVISION FOR VARIABLE INPUT
  AND OUTPUT TAPE NUMBERS.  PRESENT COPY HAS INPUT (NRIP) = 5 AND
  OUTPUT (NROP) = 6.  WITHIN THE PROGRAM THE LIBRATION TENSOR
  IS REFERRED TO CHIEFLY AS R OR OMEGA AND ONLY OCCASIONALLY AS L,
  THE SYMBOL USED IN THE PAPER DESCRIBING THE METHOD.
  HOWEVER, ALL OUTPUT LABELS HAVE BEEN CHANGED TO L RATHER THAN R.
  NOTE THAT ATOMIC WEIGHTS (OPTIONAL) ARE USED ONLY TO CALCULATE
  CENTER OF MASS AND NOT AT PRESENT TO WEIGHT THE OBSERVATIONAL
  EQUATIONS IN SETTING UP NORMAL EQUATIONS.  THUS L AND REDUCED T,
  S, AND OTHER RESULTS ARE INDEPENDENT OF ATOMIC WEIGHTS AT
  PRESENT.  TRACE OF S IS SET = 0 (AND NECESSARILY REMAINS SO).
  S(3,3) IS AUTOMATICALLY DELETED IF NO DELETION IS SPECIFIED BY
  NOT(I), TO PERMIT SOLVING NORMAL EQUATIONS, BUT THIS IS LATER
  SUPERSEDED BY THE CONDITION TRACE OF S = 0.

  IN THIS VERSION PROVISION FOR HANDLING SITE-SYMMETRY
  AUTOMATICALLY IS INCLUDED ONLY FOR MOLECULES AT CENTROSYMMETRIC
  SITES (SPECIFIED BY NSYM = 2).  OTHER SITE-SYMMETRIES MAY BE
  HANDLED AUTOMATICALLY LATER BY EXTENDING THE RANGE OF NSYM.

THE COMPLETE PROGRAM CONSISTS OF THE MAIN ROUTINE (THIS DECK) AND
 THREE SUBROUTINES, TWMT, MATINV, AND EIGEN.  TWMT FORMS THE
 21-BY-21 MATRIX OF THE NORMAL EQUATIONS.  MATINV SOLVES THE
 NORMAL EQUATIONS, AND GIVES THE INVERSE OF THE MATRIX OF THE
 NORMAL EQUATIONS AS WELL AS THE SOLUTION VECTOR.  EIGEN CALCU-
 LATES THE EIGENVALUES AND EIGENVECTORS OF A 3-BY-3 MATRIX.
SUBROUTINE KAY CALCULATES INTERATOMIC DISTANCES CORRECTED FOR
MOLECULAR DILATION (NOTE MANY OF THE DISTANCES PRODUCED ARE
MEANINGLESS).

INPUT DATA MUST BE IN THE FOLLOWING FORMATS AND SEQUENCE.
```

1. FORMAT(I5,10A6) PARAMETER SET NUMBER AND IDENTIFYING MESSAGE.
MAKE THE IDENTIFYING NUMBER NEGATIVE TO GET PUNCHED OUTPUT
OF ORTHOGONALIZED COORDINATES AND DELTA U,S

2. FORMAT(6F10.3,8I2,I4) FIRST SIX QUANTITIES ARE A,B,C,ALPHA,BETA
GAMMA IN ANGSTROMS,DEGREES RESPECTIVELY.

(61-62)NTL = TOTAL NUMBER OF ATOMS IN THE CALCULATION. THIS MAY BE
LARGER THAN THE NUMBER IN THE RIGID BODY IF ONE WISHES TO GET
PRINCIPAL AXES OF SOME VIBRATION ELLIPSOIDS WITHOUT INCLUDING
CORRESPONDING ATOMS IN RIGID BODY.

(63-64)NATOM = NUMBER OF ATOMS IN THE RIGID BODY.

(65-66)NORIG. IF THIS PARAMETER IS SET = 0, POSITIONS OF FIRST NATOM
ATOMS WILL BE AVERAGED (WITH APPROPRIATE WEIGHTS, IF GIVEN AS
SPECIFIED IN 4 BELOW) TO GET ORIGIN FOR CALCULATION. IF NORIG
NOT EQUAL TO ZERO, ORIGIN IS TO BE READ IN (SEE 5. BELOW).

(67-68)NSYM. IF NSYM = 1, NO SITE-SYMMETRY ASSUMED. IF NSYM = 2,
MOLECULAR SITE ASSUMED TO BE CENTROSYMMETRIC.

(69-70)NMAT. IF NMAT = 0, MATRIX OF NORMAL EQUATIONS AND ITS INVERSE
ARE NOT PRINTED OUT. IF NMAT NOT EQUAL TO ZERO, THEY ARE OUTPUT

(71-72)NSPAX. IF THIS VARIABLE IS NOT EQUAL TO ZERO, A SPECIAL AXIAL
SYSTEM IS TO BE READ IN ON THREE FOLLOWING CARDS AND T,L, AND
SOME OTHER QUANTITIES WILL BE REFERRED TO THESE AXES. THIS
OPTION IS USEFUL IF ONE WISHES TO EXAMINE RESULTS IN A SPECIAL
AXIAL SYSTEM, E.G., THE INERTIAL AXES OF THE MOLECULE.
IF NSPAX = 0, NO SPECIAL AXES TO BE INPUT.
NOTE THAT THIS SPECIAL AXIS SYSTEM IS NOT USED IN THE LEAST
SQUARES ANLYSIS,BUT RESULTS ARE TRANSFORMED TO IT AT THE
(END OF CALCULATIONS? FJH)

(73-74) NFUZZ, THE NUMBER OF BETAS IN INPUT RELATED TO OTHERS
BY SYMMETRY. THUS THE NUMBER OF INDEPENDENT BETAS
IN LEAST-SQUARES IS 6*NATOM - NFUZZ

(75-76) NRATS
NRATS=0 NORMALLY -- INPUT BETAS FROM FLINUS OUTPUT.
NRATS= -1 NORMAL OPERATION WITH INPUT U'S.
NRATS = -2 NORMAL OPERATION WITH INPUT B'S.
NRATS = +1 INPUT U'S WITH A CALL TO RATS
NRATS = +2 INPUT B'S WITH A CALL TO RATS
NRATS = +3 INPUT BETAS WITH A CALL TO RATS
IF NRATS GREATER THAN ZERO A SPECIAL RATS INPUT CARD (6A)
MUST FOLLOW THE PARAMETER CARDS. (SEE BELOW)

(77-80) NKAY - THE MAXIMUM NUMBER OF INTERATOMIC DISTANCES
TO BE CALCULATED (CORRECTED FOR RIGID BODY MOTION)

3. (OPTIONAL. PRESENT ONLY IF NSPAX NOT EQUAL TO ZERO).
THREE CARDS, EACH FORMAT (3F10.7), AND EACH CONTAINING DIRECTION
COSINES OF ONE AXIS OF THE SPECIAL AXIAL SYSTEM. NOTE THAT THESE
DIRECTION COSINES MUST BE REFERRED TO THE ORTHOGONALIZED AXIAL
SYSTEM SPECIFIED IN THE COMMENTS AT THE START.

4,5. ATOM PARAMETER CARDS IN B+L FORMAT
TWO CARDS PER ATOM

CARD 4 (A6,21X,4F9.6) ATOM NAME, POSITION PARAMETERS (X,Y,Z), AND RELATIVE WEIGHTS OF THE NATOM ATOMS OF THE RIGID BODY AND POSITION PARAMETERS OF THE (NTL - NATOM) REMAINING ATOMS. (NTL-NATOM) BLANK CARDS MAY BE USED IN PLACE OF POSITIONS OF THE ATOMS NOT IN THE RIGID BODY. NO USE IS MADE OF THEM, BUT CORRESPONDING U"S WILL BE OUTPUT IF B"S ARE INCLUDED. IF ATOMIC WEIGHTS ARE OMITTED, OR IF THEY ARE PUNCHED AS 0.0, THE PROGRAM WILL ASSIGN WEIGHT 1.0 TO ALL SUCH ATOMS. THIS FIELD CAN NORMALLY BE IGNORED UNLESS THE POSITION OF THE CENTER OF MASS (AS DISTINCT FROM THE CENTROID) IS WANTED. AS MENTIONED ABOVE THE NORMAL EQUATIONS ARE NOT NOW WEIGHTED.

CARD 5 - FORMAT(6F9.6) VIBRATION ELLIPSOID PARAMETERS FOR ALL ATOMS. ONE ATOM PER CARD, WITH B"S IN ORDER B11,B22,B33,B12,B13,B23. NOTE INTRINSIC FACTOR OF 2 IN B(IJ), MENTIONED IN COMMENTS ABOVE.

CARDS 4 AND 5 OF ATOM SET ALTERNATE AS IN FLINUS

6A. FORMAT(3I3) OPTIONAL - ONLY IF NRATS IS POSITIVE.
SUPPLY THREE ATOM NUMBERS. AN ORTHOGONAL COORINDATE SYSTEM WILL BE SET UP BASED ON THESE THREE ATOMS. IF THE POSITIONS OF THE ATOMS ARE R(I1), R(I2), AND R(I3) (VECTORS) THEN THE AXIS SYSTEM IS

A(1) = (R(I2) - R(I1))
A(2) = A(1) X (R(I3) - R(I1))
A(3) = A(1) X A(2)

THE AXES ARE THEN NORMALIZED TO UNIT LENGTH. ALL SUBSEQUENT ANALYSIS IN TLS6 IS CARRIED OUT REFERRING TO THIS SYSTEM AS THE 'ORIGINAL' AXIS SYSTEM.

6. (OPTIONAL. PRESENT ONLY IF NORIG NOT EQUAL TO ZERO). ONE CARD, FORMAT (3F10.8), X,Y,Z FOR ASSUMED ORIGIN.

7. FORMAT(21 I3). (NOT(I), I = 1,21). THIS IS A SINGLE CARD CONTAINING DELETION SPECIFICATIONS FOR THE MATRIX OF NORMAL EQUATIONS. SEE THE PAPER FOR DISCUSSION OF TERMS WHICH VANISH AS A CONSEQUENCE OF SITE-SYMMETRY. IDENTIFY THE TERM(S) WHOSE ROW AND COLUMN ARE TO BE DELETED BY THE NUMBER(S) IN THE FOLLOWING LIST, AND ENTER THE NUMBER(S) WITH UNITS PLACES IN COLUMNS 3,6,9,.... SKIP NO FIELDS. AS SOON AS PROGRAM FINDS AN EMPTY FIELD IT WILL NOT LOOK BEYOND THAT POINT.

T11	1	L11	7	S11	13	S23	16
T22	2	L22	8	S22	14	S31	17
T33	3	L33	9	S33	15	S12	18
T12	4	L12	10			S32	19
T13	5	L13	11			S13	20
T23	6	L23	12			S21	21

NOTE THAT IF NO TERMS ARE TO BE DELETED THERE MUST BE A BLANK CARD HERE, OR AT LEAST ONE WHICH IS BLANK IN COLUMNS 1-3. THE PROGRAM WILL AUTOMATICALLY DELETE S33 IF (AND ONLY IF) NO DELETIONS ARE HERE SPECIFIED. ONE DIAGONAL ELEMENT OF S MUST BE DELETED. WHEN NSYM = 2, THE PROGRAM DELETES ALL OF S SINCE IT ASSUMES THE SITE IS CENTROSYMMETRIC.

8. FORMAT (3I3). NDA,NCS,NIA. SPECIFICATIONS FOR RESETTING DELETED TERMS WHEN TWO TERMS ARE RELATED BY SYMMETRY. THE NUMBERING SYSTEM IS THE SAME AS THAT IN 7. NDA IS THE NUMBER OF THE TERM WHICH WAS DELETED. NIA IS THE NUMBER OF THE TERM TO WHICH IT IS RELATED BY SYMMETRY. NCF IS THE FACTOR RELATING THE

TWO, EXPRESSED IN THE INTEGER MODE. IF, FOR EXAMPLE, S12 = S21 AND S21 HAD BEEN DELETED (ROW 21, COLUMN 21), THEN ONE CARD WOULD BE NEEDED HERE, WITH 21 IN COLS 2,3, 1 IN COL 6, AND 18 IN COLS 8,9.
ONE CARD IS NEEDED FOR EACH TERM TO BE RESET, AND THE FINAL SUCH CARD MUST BE FOLLOWED BY A BLANK. IF NO TERMS ARE TO BE RESET, ONE BLANK CARD MUST BE HERE.

9. CALCULATION FOR ANOTHER COMPOUND MAY BE DONE MERELY BY FOLLOWING THE LAST CARD OF ONE GROUP BY THE FIRST CARD OF THE NEXT, WITH NO BLANKS INTERSPERSED, OTHER THAN THOSE NORMALLY CORRESPONDING TO 7. AND 8. ABOVE. TO EXIT, FOLLOW THE CARD SPECIFIED IN 8. BY TWO BLANKS.

TØRSIØN

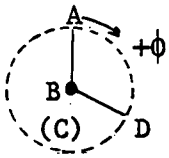
BROOKHAVEN CRYSTALLOGRAPHIC COMPUTER PROGRAM

PRØGRAM TØRSIØN(INPUT,ØUTPUT,TAPE8=INPUT,TAPE9=ØUTPUT,TAPE1=ØUTPUT)
FL=17K; TIME: Fast (≈ 1 sec on the CDC 6600 for a small amino acid)

A program for the calculation of torsion angles by G. L. Gartland (University of Pittsburgh) and modified by R. Shiono.

Given a set of four points A, B, C and D in space, the torsion angle ABCD is defined as the angle between the two planes formed by A, B, C and B, C, D respectively. When A, B, C and D are projected to a plane perpendicular to the line BC, along the direction from B to C, the sign of the torsion angle is defined as positive if the projected D is located within 180° clockwise rotation of A and negative otherwise. (This is the standard IUPAC-IUB definition, with $\phi = 0°$ corresponding to the cis-conformation.)

LIMITATIONS: Up to 100 Atoms. Does not provide for symmetry transformations.



This program takes the unit cell constants and a set of fractional positional parameters as input. It calculates all possible torsion angles produced by the combination of four atoms in the input set, provided all three distances A-B, B-C, and C-D are less than or equal to the maximum value specified.

The program normally calculates only the unique angles, i.e., the angle ABCD but not the DCBA which is identical to the former. But optionally the angles may be calculated and listed for an easy checking.

INPUT DATA FØRMAT

1) Title Card (20A4)
   Any alphanumeric information in columns 1-80

2) Unit Cell Constants Card (6F9.6)
   This is the common format with other programs.

Col.	1-9	10-18	19-27	28-36	27-45	46-54
	a	b	c	cos α	cos β	cos γ

   a,b,c in Å unit.

3) Control Card (3I5, F7.2)

   Col. 3-5 Number of atoms in input list (≤ 100)

Col. 10	0 (blank)	Normal (unique angles only)
	1	Calculate redundant angles
Col. 15	0 (blank)	Only positional parameter cards are used.
	1	Temperature factor cards are present in the deck (these cards will be skipped).
Col. 16-22	Maximum bonded interatomic distance (Å) to be included in the calculation of a torsion angle.	

4) Atomic Coordinate Cards (A4,A2, 21x, 3F9.6)
This is the standard coordinate card format common to all other programs (FLINUS, for example).

Col. 1-6	Any alphanumeric information for identification purposes.
Col. 28-36	x coordinate in fraction of the cell
Col. 37-45	y coordinate in fraction of the cell
Col. 46-54	z coordinate in fraction of the cell

When the temperature factor cards are interspersed in the parameter deck as in the Structure Factor programs, punch a 1 in Col. 15 of the Control Card.

OUTPUT

The distances A-B, B-C, C-D and A-D are listed as well as the torsion angles. For the redundant mode, the angle ABCD appears again as the angle DCBA.

BNL Crystallographic Computer Program

TRACER Scope

FL34K CDC 6600 Time: Short

This is a very elegant cell reduction program written by S. L. Lawton of Mobil Oil. Should be run on every unit cell to get standard setting and symmetry.

The Instructions are appended.

The usual case will be

Card 1. TITLE

Card 2. 1 0.2 for direct cell
or 2 0.2 for reciprocal cell

Card 3. Cell constants (ANGLES IN DEGREES) FØRMAT(6F10.6)

Card 4. 7

Card 5. Col 72 1

```
PROGRAM TRACER(INPUT,OUTPUT)
                              PROGRAM TRACER II

DESCRIPTION.    LATTICE TRANSFORMATION - CELL REDUCTION PROGRAM
AUTHOR,DATE.    S. L. LAWTON    (APRIL 1967)
LANGUAGE.       FORTRAN IV FOR IBM 7040

INPUT DATA

1. TITLE CARD -- FORMAT(14A5) -- ONE CARD.

      ANY ALPHANUMERIC INFORMATION DESCRIBING THE COMPOUND.  THIS
      WILL BE PRINTED BACK OUT AS A HEADING ON EACH PAGE OF OUTPUT.

2. CONTROL CARD -- FORMAT(I3,F7.3) -- ONE CARD.

      COL. 1-3   INPUT =1 CELL PARAMETERS ON PARAMETER CARD ARE IN
                          DIRECT SPACE
                       =2 CELL PARAMETERS ON PARAMETER CARD ARE IN
                          RECIPROCAL SPACE
      COL. 4-10  DEL     ABSOLUTE VALUE OF THE LARGEST PERMISSIBLE
                         DIFFERENCE BETWEEN ANY TWO OF THE SIX RE-
                         DUCED CELL SCALAR PRODUCTS.  (FOR LATTICE
                         PARAMETERS WITH E.S.D. OF 1 PART IN 10000 A.
                         DEL = 0.10 IS SATISFACTORY.  IF ABOUT 1 PART
                         IN 1000 A., DEL = 0.50 TO 1.00 MAY BE
                         NECESSARY.)
                         THIS FIELD IS IRRELAVENT IF NO CELL
                         REDUCTION IS TO BE MADE.

3. PARAMETER CARD -- FORMAT(6F10.6) -- ONE CARD

      COL. 1-10    A      LATTICE PARAMETER A (OR A*)
      COL.11-20    B      LATTICE PARAMETER B (OR B*)
      COL.21-30    C      LATTICE PARAMETER C (OR C*)
      COL.31-40  ALPHA    LATTICE PARAMETER ALPHA (OR ALPHA*)
      COL.41-50  BETA     LATTICE PARAMETER BETA  (OR BETA*)
      COL.51-60  GAMMA    LATTICE PARAMETER GAMMA (OR GAMMA*)
      (NOTE.  THE CELL EDGES ARE IN UNITS OF ANGSTROMS (IF INPUT=1)
      AND INVERSE ANGSTROMS (IF INPUT=2).  ALL ANGLES ARE IN
      DEGREES AND DECIMAL FRACTION.)

4. INSTRUCTION CARDS -- FORMAT(I3,2X,15A5).

      THESE CARDS FUNCTION AS THE COMMANDS TO THE PROGRAM IN TRANS-
      FORMING ONE CELL TO ANOTHER.  EACH CARD CONTAINS TWO ITEMS--
      AN INSTRUCTION NUMBER (NO) AND THE BRAVAIS LATTICE
      DESCRIPTION OF THE CELL ON WHICH THE PROGRAM WILL OPERATE.
      AS MANY CARDS AS ARE NECESSARY MAY BE USED TO COMPLETE THE
      DESIRED SUCCESSIVE TRANSFORMATIONS FOR ANY ONE COMPOUND.
      THEIR ORDER SPECIFIES TO THE PROGRAM THE ORDER IN WHICH THE
      TRANSFORMATIONS ARE TO BE EXECUTED.  THE LAST INSTRUCTION
      CARD FOR A PARTICULAR SEQUENCE OF TRANSFORMATIONS MUST HAVE
      NO = 7 OR 8.  BOTH MAY NOT BE PRESENT AND NEITHER MAY PRECEDE
      ANY WITH NO = 1,2,3,4,5 OR 6.  NO = 7 TRIGGERS CELL REDUCTION
      AND NO = 8 MERELY IDENTIFIES THE LAST CELL IN A SEQUENCE TO
      WHICH A TRANSFORMATION IS TO BE MADE WHEN NO CELL REDUCTION
```

IS PERFORMED. THUS, INSTRUCTION CARDS ARE READ UNTIL THE PROGRAM FINDS ONE WITH NO = 7 OR 8. INSTRUCTION CARDS WITH NO.LE.6 MAY BE INTERMIXED.

	INSTR. CODE	INSTRUCTION
COL. 3	NO = 1	TRANSFORM THIS CELL TO A NEW CELL USING A MATRIX SUPPLIED BY THE USER ON THE CORRESPONDING TRANSFORMATION CARD.
	= 2	THIS CELL IS A-CENTERED. THE PROGRAM WILL TRANSFORM IT TO A PRIMITIVE CELL USING A MATRIX IN SUBROUTINE CENTER.
	= 3	THIS CELL IS B-CENTERED. THE PROGRAM WILL TRANSFORM IT TO A PRIMITIVE CELL USING A MATRIX IN SUBROUTINE CENTER.
	= 4	THIS CELL IS C-CENTERED. THE PROGRAM WILL TRANSFORM IT TO A PRIMITIVE CELL USING A MATRIX IN SUBROUTINE CENTER.
	= 5	THIS CELL IS BODY-CENTERED. THE PROGRAM WILL TRANSFORM IT TO A PRIMITIVE CELL USING A MATRIX IN SUBROUTINE CENTER.
	= 6	THIS CELL IS FACE-CENTERED. THE PROGRAM WILL TRANSFORM IT TO A PRIMITIVE CELL USING A MATRIX IN SUBROUTINE CENTER.
	= 7	TRANSFORM THIS CELL TO ITS REDUCED CELL AND THEN IDENTIFY AND GENERATE FROM IT THE UNIT CELL OF HIGHEST SYMMETRY AND ITS CORRESPONDING LATTICE PARAMETERS. (ALL TRANSFORMATION MATRICES FOR THIS INSTRUCTION ARE GENERATED BY THE PROGRAM.)
	= 8	THIS IS A NON-EXECUTABLE INSTRUCTION NOTIFYING THE PROGRAM THAT NO TRANSFORMATION IS TO BE APPLIED TO THIS CELL. THIS INSTRUCTION CARD MAY BE USED FOR ONE OF TWO PURPOSES. (A) TO CALCULATE THE INVERSE CELL DATA OF THE INPUT PARAMETERS, VOLUME AND SIN AND COS VALUES OF CELL ANGLES, OR (B) TO IDENTIFY THE NAME OF THE CELL TO WHICH THE PREVIOUS CELL IS TRANSFORMED WHEN THE PREVIOUS CELL IN A TRANSFORMATION SEQUENCE INVOLVES ANY ONE OF THE FOLLOWING INSTRUCTIONS—NO=1,2,3,4,5 OR 6.
COL. 6-80	CELL	ANY ALPHANUMERIC INFORMATION DESCRIBING THE CELL, E.G., CRYSTAL SYSTEM AND LATTICE TYPE. LEFT JUSTIFY. THIS WILL BE PRINTED BACK OUT AS A HEADING IN THE OUTPUT FOR IDENTIFICATION PURPOSES.

5. TRANSFORMATION CARDS -- FORMAT(9F8.5).

EACH CARD CONTAINS A 3X3 TRANSFORMATION MATRIX (ONE PER CARD) TO BE USED BY THE PROGRAM FOR EACH INSTRUCTION CARD WITH NO=1 AND ARE ARRANGED IN THE SAME ORDER AS ARE THE INSTRUCTION CARDS (WITH NO=1) WHICH WILL USE THEM. IF NO INSTRUCTION CARDS ARE PRESENT WITH NO=1, THESE TRANSFORMATION CARDS ARE OMITTED.
(EXAMPLE. INSTRUCTION CARD NO. 1 HAS NO=1 AND CARD NO. 2

HAS NO=8. INSTR. CARD NO. 1 CORRESP. TO CELL NO. 1 AND INSTR. CARD NO. 2 CORRESP. TO CELL NO. 2. ONE MATRIX CARD IS THEREFORE SUPPLIED WHICH IS USED BY THE PROGRAM TO TRANSFORM CELL 1 TO CELL 2.)

THE 3X3 MATRIX FOR VECTOR TRANSFORMATION OF UNIT CELL AXES IS DEFINED BY THE USUAL CONVENTION AS FOLLOWS

```
NEWA = P(1,1)*A + P(1,2)*B + P(1,3)*C
NEWB = P(2,1)*A + P(2,2)*B + P(2,3)*C
NEWC = P(3,1)*A + P(3,2)*B + P(3,3)*C
```

WHERE A,B,C,NEWA,NEWB,NEWC ARE VECTORS DESCRIBING THE OLD AND NEW CELL RESPECTIVELY. THE ORDER OF PUNCHING IS P(1,1), P(1,2),P(1,3),P(2,1),P(2,2),P(2,3),P(3,1),P(3,2),P(3,3).

6. STOPPER CARD — 1 IN COL. 72

ANY NUMBER OF SETS OF DATA MAY BE PROCESSED WITHOUT RELOADING THE PROGRAM. EACH DATA SET CONSISTS OF ITEMS 1 - 5 ABOVE.

Notes

1. The program performs a Buerger-reduction rather than a Delauney-reduction The best reference for this procedure is Chapter 11 in "The Powder Method" by Azaroff and Buerger.

2. TRACER is, in large part, based on an AEC report IS-1411 by S. L. Lawton and R. A. Jacobson. The user desirous of full information should refer to the above report and also one by R. B. Roof Jr. published by the AEC as LA-4038.

3. The transformation matrices output by TRACER are to be used as pre-multipliers as a column vector, the elements of which may be either the real-space unit cell edge vectors or the coordinates of a point in reciprocal space. (eg. a matrix ($\underset{\sim}{M}$, say) will be provided for the transformation of cell 1 to cell 2, this may be used as follows:

$$\underset{\sim}{M}\begin{pmatrix}\vec{a}_1\\ \vec{b}_1\\ \vec{c}_1\end{pmatrix} = \begin{pmatrix}\vec{a}_2\\ \vec{b}_2\\ \vec{c}_2\end{pmatrix} \quad \text{or} \quad \underset{\sim}{M}\begin{pmatrix}h_1\\ k_1\\ \ell_1\end{pmatrix} = \begin{pmatrix}h_2\\ k_2\\ \ell_2\end{pmatrix}$$

The matrix M^{-1} for the reverse transformation is also supplied.

The basis vectors in reciprocal-space and the fractional coordinates in real-space transform under the inverse-transpose of M. i.e.

$$(\underset{\sim}{M}^{-1})^T\begin{pmatrix}\vec{a}_1^*\\ \vec{b}_1^*\\ \vec{c}_1^*\end{pmatrix} = \begin{pmatrix}\vec{a}_2^*\\ \vec{b}_2^*\\ \vec{c}_2^*\end{pmatrix} \quad \text{and} \quad (\underset{\sim}{M}^{-1})^T\begin{pmatrix}x_1\\ y_1\\ z_1\end{pmatrix} = \begin{pmatrix}x_2\\ y_2\\ z_2\end{pmatrix}$$

4. For each reduced cell examined by TRACER the corresponding Niggli matrix is provided. This is an array of the six scalar products of the real-space basis vectors for the cell. Very intelligent use of this matrix is made by the program in examining certain linear combinations of its elements for special relationships. If special relationships of unknown type (see Roof) are found, the cell is simply <u>assumed</u> to be triclinic.

   The quantity DEL, input by the user, is the largest deviation from a special value permitted by the program before fortuitous matches between these parameters are ignored.

5. It should not need stressing that TRACER concerns itself only with the dimensional symmetry of the lattice. This may be quite unrelated to the diffraction symmetry and the user should verify the presence of indicated symmetry elements by some other means.

TYPIST

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

CDC CYBER 70/74, CDC CYBER 70/76
CDC SCOPE 3.4, CDC SCOPE 2.1

PROGRAM TYPIST(I=INPUT,D=OUTPUT,L=OUTPUT,M=*,C=1,A=0)

INTRODUCTION

TYPIST IS A DOCUMENTATION PROGRAM WRITTEN BY TERRY A. CURETON OF THE CONTROL DATA CORPORATION WHILE AT BROOKHAVEN NATIONAL LABORATORY. THE CURRENT VERSION (5.0) WAS ADAPTED FROM BNL SCOPE TO SCOPE 3.4 AND SCOPE 2.0 BY H. J. BERNSTEIN. PROPER HANDLING OF 64 CHARACTERS AND OVER-PRINT CONTROL HAVE BEEN ADDED. I/O HAS BEEN RESTORED TO NORMAL FORTRAN CALLS TO ALLOW USE OF RECORD MANAGER. EXISTING DOCUMENTS NOT CONTAINING THE CHARACTER ↑ (136B ASCII, 76B DPC, SHIFT-N ON ASR-33) SHOULD BE PROCESSED WITHOUT CHANGE. THE ↑ CHARACTER NOW FLAGS OVER-PRINTING AND MUST BE USED WITH CARE.

PURPOSE

THE PURPOSE OF TYPIST IS TO PROVIDE AN EASY METHOD OF PRODUCING AND MAINTAINING DOCUMENTS. THIS IS ACCOMPLISHED BY PREPARING ON A MACHINE READABLE MEDIUM, FREE-FORM TEXT WITH INTERSPERSED CONTROL COMMANDS AND PARAMETERS FROM WHICH TYPIST CAN ASSEMBLE THE PAGES OF A FINISHED DOCUMENT. WHEN PRINTED ON LINE PRINTER PAGES, THE OUTPUT IS SUITABLE FOR DIRECT USE AS A FORMAL DOCUMENT BY LIMITING TO 80 COLS. PER LINE, CUTTING TO THE STANDARD TYPEWRITER PAGE SIZE, BURSTING AND STAPLING.

TYPIST HAS THE CAPABILITY FOR SELECTIVE PROCESSING OF PORTIONS OF TEXT WITHIN A DOCUMENT AND OF WHOLE DOCUMENTS ON A MULTI-DOCUMENT FILE UNDER CONTROL OF PARAMETERS SUPPLIED ON THE PROGRAM CALL. THIS MAKES THE PROGRAM SUITABLE FOR MAINTAINING AN ENTIRE LIBRARY OF DOCUMENTS RETRIEVABLE BY NAME OR CHARACTERISTICS.

THE EASE WITH WHICH CHANGES CAN BE MADE TO THE DOCUMENT LAYOUT AND CONTENTS PROVIDES AN EFFECTIVE MEANS OF UPDATING AND PRODUCING DOCUMENTS WHICH CHANGE FREQUENTLY. THE PROCESS PARTICULARILY LENDS ITSELF TO COMPUTERIZED FILE EDITING METHODS SUCH AS THE INTERCOM EDITOR, SCOPE UPDATE, OR OTHER FILE MAINTENANCE SYSTEMS.

DESCRIPTION

TYPIST IS A CDC 6600/7600 PROGRAM WRITTEN ENTIRELY IN FORTRAN AND COMPILED AND OPTIMIZED BY THE FORTRAN EXTENDED 4 COMPILER. THE PROGRAM REQUIRES A MINIMUM OF 50K(OCTAL) WORDS OF CENTRAL MEMORY STORAGE FOR EXECUTION. USE OF THE INDEXING FEATURE WILL INCREASE THIS REQUIREMENT SLIGHTLY ACCORDING TO THE VOLUME OF INDEX TEXT STORED. WHEN THIS FEATURE IS USED, ALL AUTOMATIC FIELD LENGTH REDUCTION MUST BE DEFEATED. IN PARTICULAR, UNDER SCOPE 2 THE CM PARAMETER SHOULD BE USED ON THE JOB CARD. THE AMOUNT OF STORAGE USED, THE OUTPUT PAGE COUNT, AND A COUNT OF ANY ERRORS DETECTED IS DISPLAYED IN A DAYFILE MESSAGE FOR EACH DOCUMENT. THE PROGRAM IS AVAILABLE AT BNL AS A RELOCATABLE PROGRAM ON THE PERMANENT FILE TYPIST,ID=CPROGS.

PROGRAM CALL

THE TYPIST PROGRAM CALL USES FREE-FORM PARAMETERS SIMILAR TO THOSE USED BY FTN. THE POSSIBLE PARAMETERS AND THEIR DEFAULTS ARE:

TYPIST(I=INPUT,D=OUTPUT,L=OUTPUT,M=*,C=1,A=0)

-FORM-	-EXPLANATION-
I=LFN1	DEFINES INPUT DATA FILE.
D/E=LFN2	DEFINES CONTENT AND DESTINATION OF DIAGNOSTIC OUTPUT. IF D IS SPECIFIED, ALL INPUT LINES AND MESSAGES ARE PRINTED. IF E IS SPECIFIED, ONLY LINES WITH ERROR/WARNING MESSAGES APPEAR.
L=LFN3	DEFINES DESTINATION OF DOCUMENT OUTPUT.
M/S=*	DEFINES THE MASTER CHARACTER (*) AND/OR SELECT MODE. IN SELECT MODE (S=), ALL INPUT LINES TO BE PROCESSED BY TYPIST MUST CONTAIN THE MASTER CHARACTER IN COLUMN 1. IN NORMAL MODE (M=), ONLY TYPIST COMMANDS REQUIRE THE MASTER CHARACTER AND ALL OTHER LINES ARE CONSIDERED AS TEXT.
C=N	SPECIFIES INITIAL NUMBER OF COPIES OF EACH DOCUMENT TO PRODUCE BY SERIALLY COPYING WHOLE DOCUMENT TO LFN3. USE OF *COPY COMMANDS WITHIN A DOCUMENT WILL INCREASE THE NUMBER OF COPIES OF THAT DOCUMENT ONLY.
A=N	SPECIFIES THE NUMBER OF ERRORS ALLOWED BEFORE SUPPRESSING MULTIPLE COPIES. THIS MAY BE USED TO OVERRIDE THE SAFETY PRECAUTION WHEN ERRORS ARE FOUND IN TYPIST COMMANDS.

O=OPTION THIS PARAMETER MAY BE USED TO SELECT PORTIONS OF THE INPUT FILE TO PROCESS AS DEFINED BY *OPTION AND *DOC COMMANDS WITHIN IT. THIS PARAMETER MAY BE REPEATED TO TURN ON MULTIPLE OPTIONS AND/OR SELECT SEVERAL DOCUMENTS FROM A MULTI-DOCUMENT INPUT FILE. THE O= PREFIX MAY BE OMITTED IF THE OPTION NAME DOES NOT CONFLICT WITH OTHER PROGRAM CALL PARAMETERS. (UNRECOGNIZED PARAMETERS ARE OPTIONS.)

INPUT DATA

THE INPUT FILE CONSISTS OF A MIXTURE OF CONTROL COMMANDS AND TEXT DATA IN LINES OF UP TO 135 CHARACTERS (DYNAMICALLY CONTROLLED BY THE *SIZE COMMAND).

THE SELECT MODE OF OPERATION SPECIFIED BY THE S=* PARAMETER PROVIDES TYPIST THE ABILITY TO REPROCESS OTHER PROGRAM-S INPUT WITHOUT CHANGES OR CONFLICTS. IN THIS MODE TYPIST ONLY LOOKS AT INPUT LINES BEGINNING WITH THE SPECIFIED MASTER CHARACTER. IF THE OTHER PROGRAM IGNORES THESE LINES, SUCH AS COMMENT LINES IN COMPILER/ASSEMBLER INPUT, THERE IS NO CONFLICT EITHER WAY. ANOTHER USE IS TO BUILD A TYPIST INPUT FILE WITH SEVERAL DIFFERENT MASTER CHARACTERS USED, AND SELECT INPUT WITH EACH, ONE PER RUN. THIS FEATURE EXISTS OUTSIDE AND SEPARATE FROM THE SELECTIVE PROCESSING PROVIDED BY THE OPTION PARAMETERS AND COMMANDS.

A CONTROL COMMAND IS DEFINED AS A LINE BEGINNING WITH THE MASTER CONTROL CHARACTER (M/S=* PARAMETER) IN COLUMN 1. IMMEDIATELY FOLLOWED BY A COMMAND NAME WHICH IS TERMINATED BY A NON-ALPHABETIC CHARACTER SUCH AS A DIGIT, BLANK OR SPECIAL CHARACTER. LINES WHICH DO NOT MEET THESE CRITERIA ARE CONSIDERED TEXT DATA. A COMMAND NAME MAY BE ENTERED IN IT,S ENTIRETY OR IT,S TWO-LETTER ABBREVIATION MAY BE USED FOR COMPACTNESS. TABLE 1 IS A LIST OF THE COMMAND SET WITH NOTES ON USAGE.

CERTAIN COMMANDS ACCEPT NUMERIC AND/OR TEXT ENTRIES FOLLOWING THE COMMAND. THE FOLLOWING CONVENTIONS APPLY:

1) WHEN PRESENT, THE TERMINATING COMMA IS PART OF THE ENTRY AND MAY BE USED ALONE TO INDICATE AN UNSPECIFIED OR DEFAULT ENTRY.

2) MULTIPLE BLANKS MAY PRECEED OR FOLLOW AN ENTRY AND IT-S COMMA.

3) A NUMERIC ENTRY IS DEFINED AS A CONSECUTIVE SERIES OF NUMERIC DIGITS TERMINATED BY A NON-NUMERIC CHARACTER.

4) A MIXED NUMBER IS DEFINED AS A CONSECUTIVE SERIES OF UP TO 10 NON-BLANK CHARACTERS ENDING WITH AT LEAST ONE DIGIT AND FOLLOWED BY A COMMA AND/OR BLANK. (USED BY *PAGE COMMAND.)

5) A NAME ENTRY CONSIST OF UP TO 8 NON-BLANK CHARACTERS TERMINATED BY A COMMA AND/OR BLANK. (USED WITH SELECTIVE PROCESSING OPTION NAMES.)

6) A PHRASE ENTRY IS A TEXT STRING ALL ON ONE LINE WHICH IS STRUCTURED BY SLASHES AND TERMI

TYPIST

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

CDC CYBER 70/74, CDC CYBER 70/76
CDC SCOPE 3.4, CDC SCOPE 2.1

PROGRAM TYPIST(I=INPUT,D=OUTPUT,L=OUTPUT,M=*,C=1,A=0)

INTRODUCTION

TYPIST IS A DOCUMENTATION PROGRAM WRITTEN BY TERRY A. CURETON OF THE CONTROL DATA CORPORATION WHILE AT BROOKHAVEN NATIONAL LABORATORY. THE CURRENT VERSION (5.0) WAS ADAPTED FROM BNL SCOPE TO SCOPE 3.4 AND SCOPE 2.0 BY H. J. BERNSTEIN. PROPER HANDLING OF 64 CHARACTERS AND OVER-PRINT CONTROL HAVE BEEN ADDED. I/O HAS BEEN RESTORED TO NORMAL FORTRAN CALLS TO ALLOW USE OF RECORD MANAGER. EXISTING DOCUMENTS NOT CONTAINING THE CHARACTER ↑ (136B ASCII, 76B DPC, SHIFT-N ON ASR-33) SHOULD BE PROCESSED WITHOUT CHANGE. THE ↑ CHARACTER NOW FLAGS OVER-PRINTING AND MUST BE USED WITH CARE.

PURPOSE

THE PURPOSE OF TYPIST IS TO PROVIDE AN EASY METHOD OF PRODUCING AND MAINTAINING DOCUMENTS. THIS IS ACCOMPLISHED BY PREPARING ON A MACHINE READABLE MEDIUM, FREE-FORM TEXT WITH INTERSPERSED CONTROL COMMANDS AND PARAMETERS FROM WHICH TYPIST CAN ASSEMBLE THE PAGES OF A FINISHED DOCUMENT. WHEN PRINTED ON LINE PRINTER PAGES, THE OUTPUT IS SUITABLE FOR DIRECT USE AS A FORMAL DOCUMENT BY LIMITING TO 80 COLS. PER LINE, CUTTING TO THE STANDARD TYPEWRITER PAGE SIZE, BURSTING AND STAPLING.

TYPIST HAS THE CAPABILITY FOR SELECTIVE PROCESSING OF PORTIONS OF TEXT WITHIN A DOCUMENT AND OF WHOLE DOCUMENTS ON A MULTI-DOCUMENT FILE UNDER CONTROL OF PARAMETERS SUPPLIED ON THE PROGRAM CALL. THIS MAKES THE PROGRAM SUITABLE FOR MAINTAINING AN ENTIRE LIBRARY OF DOCUMENTS RETRIEVABLE BY NAME OR CHARACTERISTICS.

THE EASE WITH WHICH CHANGES CAN BE MADE TO THE DOCUMENT LAYOUT AND CONTENTS PROVIDES AN EFFECTIVE MEANS OF UPDATING AND PRODUCING DOCUMENTS WHICH CHANGE FREQUENTLY. THE PROCESS PARTICULARILY LENDS ITSELF TO COMPUTERIZED FILE EDITING METHODS SUCH AS THE INTERCOM EDITOR, SCOPE UPDATE, OR OTHER FILE MAINTENANCE SYSTEMS.

DESCRIPTION

TYPIST IS A CDC 6600/7600 PROGRAM WRITTEN ENTIRELY IN FORTRAN AND COMPILED AND OPTIMIZED BY THE FORTRAN EXTENDED 4 COMPILER. THE PROGRAM REQUIRES A MINIMUM OF 50K(OCTAL) WORDS OF CENTRAL MEMORY STORAGE FOR EXECUTION. USE OF THE INDEXING FEATURE WILL INCREASE THIS REQUIREMENT SLIGHTLY ACCORDING TO THE VOLUME OF INDEX TEXT STORED. WHEN THIS FEATURE IS USED, ALL AUTOMATIC FIELD LENGTH REDUCTION MUST BE DEFEATED. IN PARTICULAR, UNDER SCOPE 2 THE CM PARAMETER SHOULD BE USED ON THE JOB CARD. THE AMOUNT OF STORAGE USED, THE OUTPUT PAGE COUNT, AND A COUNT OF ANY ERRORS DETECTED IS DISPLAYED IN A DAYFILE MESSAGE FOR EACH DOCUMENT. THE PROGRAM IS AVAILABLE AT BNL AS A RELOCATABLE PROGRAM ON THE PERMANENT FILE TYPIST,ID=CPROGS.

PROGRAM CALL

THE TYPIST PROGRAM CALL USES FREE-FORM PARAMETERS SIMILAR TO THOSE USED BY FTN. THE POSSIBLE PARAMETERS AND THEIR DEFAULTS ARE:

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TYPIST(I=INPUT,D=OUTPUT,L=OUTPUT,M=*,C=1,A=0)
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-FORM-	-EXPLANATION-
I=LFN1	DEFINES INPUT DATA FILE.
D/E=LFN2	DEFINES CONTENT AND DESTINATION OF DIAGNOSTIC OUTPUT. IF D IS SPECIFIED, ALL INPUT LINES AND MESSAGES ARE PRINTED. IF E IS SPECIFIED, ONLY LINES WITH ERROR/WARNING MESSAGES APPEAR.
L=LFN3	DEFINES DESTINATION OF DOCUMENT OUTPUT.
M/S=*	DEFINES THE MASTER CHARACTER (*) AND/OR SELECT MODE. IN SELECT MODE (S=), ALL INPUT LINES TO BE PROCESSED BY TYPIST MUST CONTAIN THE MASTER CHARACTER IN COLUMN 1. IN NORMAL MODE (M=), ONLY TYPIST COMMANDS REQUIRE THE MASTER CHARACTER AND ALL OTHER LINES ARE CONSIDERED AS TEXT.
C=N	SPECIFIES INITIAL NUMBER OF COPIES OF EACH DOCUMENT TO PRODUCE BY SERIALLY COPYING WHOLE DOCUMENT TO LFN3. USE OF *COPY COMMANDS WITHIN A DOCUMENT WILL INCREASE THE NUMBER OF COPIES OF THAT DOCUMENT ONLY.
A=N	SPECIFIES THE NUMBER OF ERRORS ALLOWED BEFORE SUPPRESSING MULTIPLE COPIES. THIS MAY BE USED TO OVERRIDE THE SAFETY PRECAUTION WHEN ERRORS ARE FOUND IN TYPIST COMMANDS.

O=OPTION THIS PARAMETER MAY BE USED TO SELECT PORTIONS OF THE INPUT FILE TO PROCESS AS DEFINED BY *OPTION AND *DOC COMMANDS WITHIN IT. THIS PARAMETER MAY BE REPEATED TO TURN ON MULTIPLE OPTIONS AND/OR SELECT SEVERAL DOCUMENTS FROM A MULTI-DOCUMENT INPUT FILE. THE O= PREFIX MAY BE OMITTED IF THE OPTION NAME DOES NOT CONFLICT WITH OTHER PROGRAM CALL PARAMETERS. (UNRECOGNIZED PARAMETERS ARE OPTIONS.)

INPUT DATA

THE INPUT FILE CONSISTS OF A MIXTURE OF CONTROL COMMANDS AND TEXT DATA IN LINES OF UP TO 135 CHARACTERS (DYNAMICALLY CONTROLLED BY THE *SIZE COMMAND).

THE SELECT MODE OF OPERATION SPECIFIED BY THE S=* PARAMETER PROVIDES TYPIST THE ABILITY TO REPROCESS OTHER PROGRAM-S INPUT WITHOUT CHANGES OR CONFLICTS. IN THIS MODE TYPIST ONLY LOOKS AT INPUT LINES BEGINNING WITH THE SPECIFIED MASTER CHARACTER. IF THE OTHER PROGRAM IGNORES THESE LINES, SUCH AS COMMENT LINES IN COMPILER/ASSEMBLER INPUT, THERE IS NO CONFLICT EITHER WAY. ANOTHER USE IS TO BUILD A TYPIST INPUT FILE WITH SEVERAL DIFFERENT MASTER CHARACTERS USED, AND SELECT INPUT WITH EACH, ONE PER RUN. THIS FEATURE EXISTS OUTSIDE AND SEPARATE FROM THE SELECTIVE PROCESSING PROVIDED BY THE OPTION PARAMETERS AND COMMANDS.

A CONTROL COMMAND IS DEFINED AS A LINE BEGINNING WITH THE MASTER CONTROL CHARACTER (M/S=* PARAMETER) IN COLUMN 1. IMMEDIATELY FOLLOWED BY A COMMAND NAME WHICH IS TERMINATED BY A NON-ALPHABETIC CHARACTER SUCH AS A DIGIT, BLANK OR SPECIAL CHARACTER. LINES WHICH DO NOT MEET THESE CRITERIA ARE CONSIDERED TEXT DATA. A COMMAND NAME MAY BE ENTERED IN IT,S ENTIRETY OR IT,S TWO-LETTER ABBREVIATION MAY BE USED FOR COMPACTNESS. TABLE 1 IS A LIST OF THE COMMAND SET WITH NOTES ON USAGE.

CERTAIN COMMANDS ACCEPT NUMERIC AND/OR TEXT ENTRIES FOLLOWING THE COMMAND. THE FOLLOWING CONVENTIONS APPLY:

1) WHEN PRESENT, THE TERMINATING COMMA IS PART OF THE ENTRY AND MAY BE USED ALONE TO INDICATE AN UNSPECIFIED OR DEFAULT ENTRY.

2) MULTIPLE BLANKS MAY PRECEED OR FOLLOW AN ENTRY AND IT-S COMMA.

3) A NUMERIC ENTRY IS DEFINED AS A CONSECUTIVE SERIES OF NUMERIC DIGITS TERMINATED BY A NON-NUMERIC CHARACTER.

4) A MIXED NUMBER IS DEFINED AS A CONSECUTIVE SERIES OF UP TO 10 NON-BLANK CHARACTERS ENDING WITH AT LEAST ONE DIGIT AND FOLLOWED BY A COMMA AND/OR BLANK. (USED BY *PAGE COMMAND.)

5) A NAME ENTRY CONSIST OF UP TO 8 NON-BLANK CHARACTERS TERMINATED BY A COMMA AND/OR BLANK. (USED WITH SELECTIVE PROCESSING OPTION NAMES.)

6) A PHRASE ENTRY IS A TEXT STRING ALL ON ONE LINE WHICH IS STRUCTURED BY SLASHES AND TERMINATED BY A COMMA. (USED BY THE INDEXING FEATURE.)

7) AN INPUT TEXT SEGMENT IS FREE-FORM AND DEFINED AS ALL CHARACTERS FROM THE FIRST TO LAST NON-BLANK ON ONE LINE.

DIAGNOSTIC OUTPUT

THE DIAGNOSTIC OUTPUT PRODUCED BY TYPIST MAY BE DIRECTED TO ANY FILE INCLUDING THE DOCUMENT OUTPUT FILE. THE DIAGNOSTIC OUTPUT WILL PRECEED EACH DOCUMENT WHEN DIRECTED TO THE SAME FILE. THE DIAGNOSTIC OUTPUT CONTAINS IN NORMAL MODE (D=LFN2), ALL PROCESSED INPUT LINES AND ANY ERROR/WARNING MESSAGES PRODUCED. ANY INPUT LINES NOT PROCESSED THRU USE OF THE SELECT MODE OR SKIPPED VIA *OPTION OR DOCUMENT SELECTION WILL NOT APPEAR IN THE DIAGNOSTIC OUTPUT. IN SHORTENED OUTPUT MODE (E=LFN2), ONLY LINES WITH ASSOCIATED MESSAGES ARE PRODUCED. THE LINES IN THIS OUTPUT ARE ONE CHARACTER (CARRIAGE CONTROL) LONGER THAN THE INPUT LINES REGARDLESS OF THE *SIZE PARAMETER. THUS, UPDATE LINE IDENTIFIERS IN THE INPUT ARE VISIBLE EVEN THOUGH A *SIZE COMMAND MAY CAUSE TYPIST TO IGNORE THEM.

THE BASIC APPROACH TO HANDLING ERRORS DETECTED BY TYPIST IS TO CONTINUE PROCESSING IF AT ALL POSSIBLE. IN CERTAIN SITUATIONS IT IS NECESSARY FOR MINIMAL CORRECTIVE ACTION TO BE TAKEN IN ORDER TO CONTINUE. THERE ARE NO PROGRAM STOPS IN TYPIST AND ONLY TWO TYPES OF ABORT, ONE IS ON A TYPIST CALL ERROR, AND THE OTHER IS ON AN IO ERROR ON A FILE. BOTH EXIT VIA ABT AND ARE ACCOMPANIED BY A DAYFILE MESSAGE. IN ADDITION, A MODE-1 ERROR WILL OCCUR IF TYPIST RUNS OUT OF CORE STORAGE.

ERROR AND WARNING MESSAGES FOLLOW THE LINE REFERRED TO AND ARE FOLLOWED BY A BLANK LINE TO MAKE THEM MORE NOTICEABLE. A COUNT OF THE ERRORS DETECTED IS MAINTAINED AND INCLUDED IN THE DAYFILE MESSAGE FOR EACH DOCUMENT. IF THE COUNT IS GREATER THAN THE ERROR ALLOWANCE PARAMETER (A=N), MULTIPLE COPIES WILL BE SUPPRESSED.

DOCUMENT OUTPUT

THE OUTPUT DIRECTED BY THE L=LFN3 PARAMETER CONTAINS PAGES OF TEXT CONSISTING OF 62 LINES OF UP TO 135 COLUMNS EACH PLUS A CARRIAGE CONTROL CHARACTER. THIS MAY BE CONTROLLED DYNAMICALLY BY THE *LIMIT COMMAND. CHARACTERS WITHIN A LINE MAY BE OVER-PRINTED REPEATLY TO BE DARKENED BY THE *BOLD COMMAND, AND BY THE ↑CHARACTER (136B ASCII, 76B DPC, SHIFT-N ON TTY), WHICH CAUSES THE FOLLOWING CHARACTER TO BE OVER-PRINTED. A STRING OF N ↑ CHARACTERS CAUSES THE NEXT CHARACTER TO BE PRINTED N+1 TIMES IN THE SAME PLACE. IF THE NEXT CHARACTER IS BLANK, AND ↑ IS PRINTED N TIMES. FOR THE CONVENIENCE OF USERS WHO WISH TO DISPLAY TYPIST OUTPUT TEXT ON DEVICES WHICH ARE SLOW OR HAVE SHORT LINES, TRAILING BLANKS ARE TRIMMED TO A 6600 WORD (10 CHARACTERS).

MULTIPLE COPIES SPECIFIED BY THE C=N PARAMETER OR *COPY COMMANDS ARE PRODUCED SERIALLY, I.E. A WHOLE DOCUMENT AT A TIME. THE *REPEAT COMMAND MAY BE USED TO PRODUCE PARALLEL COPIES ON A PAGE BASIS BY PRINTING

MULTIPLE COPIES OF EACH PAGE TOGETHER. BECAUSE REPEATED PAGES ARE INCLUDED IN A DOCUMENT AND MAY BE RECOPIED SERIALLY, THE TOTAL NUMBER OF COPIES OF EACH PAGE IS THE PRODUCT OF THE TWO NUMBERS. A COUNT OF THE TOTAL NUMBER OF PAGES AND NUMBER OF COPIES PRODUCED APPEARS IN A DAYFILE MESSAGE AFTER EACH DOCUMENT.

FOR LARGE DOCUMENTS, PARALLEL PRINTING OF PAGES CAN MINIMIZE THE LABOR OF BURSTING AND COLLATING PAGES. FOR EXAMPLE IN MAKING 6 COPIES OF A 20 PAGE DOCUMENT: FIRST, SEPARATE INTO STRIPS, ONE PER PAGE NUMBER (20 SPLITS). THEN, OPEN OUT AND STACK ONTO A TABLE EACH STRIP FACE UP, STARTING WITH THE LAST STRIP (COLLATING). FINALLY, SPLIT OFF EACH ASSEMBLED DOCUMENT (6 SPLITS), TRIM TO SIZE, AND STAPLE. TOTALS ARE 1 COLLATING AND 26 BURSTING OPERATIONS. OF COURSE, DOCUMENTS WHICH DO NOT REQUIRE BURSTING CAN BE MOST EFFICENTLY PRODUCED SERIALLY. HOWEVER, MANY COPIES OF A LARGE DOCUMENT MAY BE MOST EFFECTIVELY PRODUCED BY A COMBINATION OF BOTH METHODS.

TEXT COMPACTER

THE TEXT COMPACTER PROVIDES THE BASIC FUNCTION OF FITTING TEXT SEGMENTS TOGETHER ON THE OUTPUT LINE, SPLITTING TEXT AT THE END OF A LINE, AND ADVANCING TO THE NEXT LINE WHEN NECESSARY. BLANK INPUT LINES ARE IGNORED BY THE TEXT COMPACTER. THE PROCESS IS WORD ORIENTED AND FOLLOWS THESE RULES:

1) IF THERE IS SUFFICENT SPACE FOR THE TEXT TO FIT BETWEEN THE CURRENT POSITION AND THE RIGHT MARGIN, THE TEXT IS TRANSFERED AND THE POSITION IS UPDATED. OTHERWISE, THE TEXT IS SPLIT AFTER THE LAST WORD WHICH WILL FIT, TRANSFERED, AND THE NEXT WORD IS POSITIONED AT THE LEFT MARGIN OF THE NEXT AVAILABLE LINE. IF NO WORD END (BLANK) IS FOUND AND THE TEXT IS TOO LONG FOR A FULL LINE, IT IS SPLIT AT THE RIGHT MARGIN. NO ATTEMPT AT HYPHENATION IS MADE (OR CONTEMPLATED). THIS PROCESS CONTINUES UNTIL THE ENTIRE TEXT STRING HAS BEEN TRANSFERED.

2) AFTER TRANSFER, THE POSITIONING CONTROL IS UPDATED TO PROVIDE ONE SPACE AFTER THE LAST CHARACTER EXCEPT WHEN THAT CHARACTER IS A PERIOD (SENTENCE END), AFTER WHICH AN ADDITIONAL SPACE IS PROVIDED. THUS, A NEW SENTENCE SHOULD ALWAYS START ON THE NEXT INPUT LINE IN ORDER TO AUTOMATICALLY GET TWO SPACES AFTER THE PERIOD.

3) WHEN A LINE ADVANCE IS REQUIRED, THE LINE SPACING CONTROL (*CONTROL COMMAND) DETERMINES THE AMOUNT OF THE ADVANCE. FIXED LINES ARE SKIPPED OVER, THUS PROTECTING THEM. SHOULD THE ADVANCE OVERFLOW THE PAGE, A NEW PAGE IS AUTOMATICALLY STARTED.

WHEN THE TEXT COMPACTER IS TURNED OFF (*PACK COMMAND) INPUT TEXT IS TRANSFERED WITHOUT ALTERATION EXCEPT FOR THE ADDITION OF A CARRIAGE CONTROL CHARACTER. HOWEVER, CONTROL COMMANDS ARE STILL OBEYED AND CAN BE USED TO PROVIDE SOME SPECIAL EFFECTS.

CONTROL COMMANDS

*PACK ON/OFF

THIS COMMAND ALLOWS THE TEXT COMPACTER TO BE SELECTIVELY TURNED OFF SO THAT INPUT TEXT CAN BE TRANSFERED LINE BY LINE WITHOUT ALTERATION. THIS ALLOWS FOR THE USE OF SPECIAL POSITIONING ARRANGEMENTS. INITIALLY THE TEXT COMPACTER IS TURNED ON.

*SIZE N

THE NUMBER OF CHARACTERS ACCEPTED PER INPUT LINE IS CONTROLLED BY THIS COMMAND. N MUST BE BETWEEN 10 AND 135. THE DEFAULT VALUE IS 80. ALL CHARACTERS FOLLOWING COLUMN N ARE IGNORED. THIS FACILITY IS REQUIRED IN ORDER TO ACCEPT FILES PREPARED BY SCOPE UPDATE OR ANY OTHER FRONT-END PROGRAM WHICH USES TRAILING IDENTIFIERS AND/OR NUMBERING.

*LIMIT N

THE OUTPUT LINE LENGTH IS CONTROLLED BY THIS COMMAND. N MUST BE BETWEEN 10 AND 135. THE DEFAULT VALUE IS 80. THIS PROVIDES A GUARANTEE THAT THE OUTPUT DOCUMENT WIDTH WILL NOT EXCEED THE LIMIT SPECIFIED, AS ALL LINE LENGTH CHECKS ARE MADE AGAINST THIS VALUE.

*COPY N

THIS PARAMETER ACCUMULATES A COUNT OF THE NUMBER OF ADDITIONAL COPIES OF THE CURRENT DOCUMENT TO BE PRODUCED. THE INITIAL NUMBER IS PROVIDED BY THE C=N PARAMETER IN THE PROGRAM CALL. MULTIPLE COPIES ARE PRODUCED SERIALLY BY COPYING THE ENTIRE DOCUMENT TO THE OUTPUT FILE A NUMBER OF TIMES. THE DEFAULT VALUE IS 1. MULTIPLE COPIES WILL BE SUPPRESSED IF THE ERROR COUNT EXCEEDS THE ERROR ALLOWANCE (A=N) PARAMETER.

*REPEAT [N]

THIS PARAMETER SETS THE NUMBER OF TIMES TO REPEAT A PAGE AND ALL SUBSEQUENT PAGES UNTIL RESET. THIS CONTROL IS DYNAMIC INSTEAD OF CUMULATIVE AND IS EFFECTED BEFORE MULTIPLE COPIES OF THE ENTIRE DOCUMENT ARE PRODUCED. CONSEQUENTLY, THE TOTAL NUMBER OF COPIES OF A PAGE IS THE PRODUCT OF THE REPEAT PARAMETER AND THE COPY COUNT. THE REPEAT FACTOR WILL BE REDUCED TO 1 WHEN THE ERROR COUNT EXCEEDS THE ERROR ALLOWANCE (A=N) PARAMETER.

*CONTROL N

THIS PARAMETER SETS THE LINE ADVANCE CONTROL USED BY THE TEXT COMPACTER TO SINGLE, DOUBLE, OR TRIPLE SPACING (N = 1, 2, OR 3). THIS WILL ALSO MODIFY THE ACTIONS OF THE *PARA COMMAND.

*MARGINS [N],[N]

THIS COMMAND DEFINES THE REFERENCE AND WORKING MARGINS USED BY THE TEXT COMPACTER. THE NUMBERS REPRESENT THE LEFT AND RIGHT MARGINS RESPECTIVELY, AND FOLLOW THE FORMAT CONVENTIONS FOR NUMERIC ENTRIES. A ZERO OR UNSPECIFIED ENTRY FOR EITHER RETAINS THE REFERENCE SETTING. THE DEFAULT MARGINS ARE POSITIONS 9 AND 80.

*INDENT [N],[N]

THIS COMMAND MOVES THE WORKING MARGINS INWARD BY THE SPECIFIED NUMBER OF POSITIONS. THE REFERENCE MARGINS SET BY DEFAULT OR THE *MARGINS COMMAND ARE NOT AFFECTED. THIS PROVIDES THE CAPABILITY FOR TEMPORARILY ADJUSTING THE MARGINS AND RESETTING TO THE REFERENCE BY A *MARGINS 0,0 COMMAND.

*TABS N1,[N2... ,N40]

THIS COMMAND DEFINES A SET OF TAB COLUMNS TO BE REFERENCED BY A *TAB COMMAND. EACH TAB COLUMN IS REFERENCED BY IT,S SEQUENCE NUMBER. I.E. THE FIRST POSITION SPECIFIED IS TAB 1, THE SECOND IS TAB 2, ETC. UP TO 40 TAB POSITIONS MAY BE SPECIFIED AND THEY SHOULD BE IN LEFT-TO-RIGHT ORDER FOR PROPER OPERATION OF THE *TAB COMMAND. EACH OCCURRENCE OF THIS COMMAND RESETS ALL OF THE TABS.

*TAB [N],[TEXT]

THIS COMMAND CAUSES THE TEXT TO BE POSITIONED AT THE NTH TAB POSITION AS DEFINED IN A PREVIOUS *TABS COMMAND. N IS THE SEQUENCE NUMBER OF THE TAB POSITION, NOT THE COLUMN NUMBER. IF N IS UNSPECIFIED OR ZERO, THE NEXT TAB POSITION PAST THE CURRENT POSITION IS SELECTED. WRAPAROUND TO THE FIRST TAB POSITION WILL OCCUR WHEN BEYOND THE RIGHTMOST TAB POSITION. IF TEXT HAS BEEN WRITTEN PAST THE SELECTED TAB POSITION, THE TEXT WILL APPEAR AT THAT POSITION IN THE NEXT AVAILABLE LINE.

FOR THIS COMMAND THE MARGINS ARE TEMPORARILY IGNORED. I.E. THE TEXT MAY START AND/OR END OUTSIDE THE MARGINS. HOWEVER, THE TEXT MUST FIT WITHIN THE LINE LIMIT AFTER POSITIONING. IT IS PERMITTED TO LEAVE POSITIONING OUTSIDE THE LEFT MARGIN FOR SUBSEQUENT TEXT POSITIONING.

*CENTER [N],TEXT

THIS COMMAND PROVIDES A MEANS TO POSITION TEXT IN THE CENTER OF A LINE OR ABOUT A SPECIFIC COLUMN. N IS THE SELECTED COLUMN NUMBER. IF N IS UNSPECIFIED OR ZERO, THE COLUMN MIDWAY BETWEEN THE MARGINS SPECIFIED BY THE *MARGINS COMMAND IS SELECTED. AS IN THE *TAB COMMAND, THE TEXT MAY START AND/OR END OUTSIDE THE MARGINS. IT NEED ONLY FIT ON THE LINE.

*RIGHT [N],TEXT

THIS COMMAND PROVIDES A MEANS TO RIGHT JUSTIFY TEXT TO A SPECIFIC COLUMN OR TO THE RIGHT MARGIN IF N IS UNSPECIFIED OR ZERO. AS WITH THE *TAB COMMAND, THE TEXT MAY START AND/OR END OUTSIDE THE MARGINS. IT NEED ONLY FIT ON THE LINE.

*LEFT [N],TEXT

THIS COMMAND WILL LEFT JUSTIFY THE TEXT TO COLUMN N. IF N IS UNSPECIFIED OR ZERO, THE LEFT MARGIN IS USED. THE TEXT MUST FIT ON THE LINE.

*SPACE [N],[TEXT]

THIS COMMAND ALLOWS INDENTING OF TEXT FROM THE CURRENT POSITION. IT MAY BE USED TO OFFSET TEXT FROM A TAB POSITION, THE LEFT MARGIN, OR THE END OF THE LAST TEXT STRING. IF N IS UNSPECIFIED OR ZERO, 1 SPACE RESULTS.

*SKIP [N],[TEXT]

THIS COMMAND PRODUCES N*INC BLANK LINES, WHERE INC IS THE *CONTROL PARAMETER, AND POSITIONS THE TEXT AT THE LEFT MARGIN OF THE NEXT AVAILABLE LINE. IF N IS UNSPECIFIED OR ZERO, ONLY A LINE ADVANCE IS EFFECTED.

*LINE [N],[TEXT]

THIS COMMAND POSITIONS THE TEXT AT THE LEFT MARGIN OF LINE N. IF N IS UNSPECIFIED OR ZERO, THE NEXT AVAILABLE LINE IS SELECTED (EQUIVALENT TO *SKIP 0). IF THE SELECTED LINE IS FIXED, A WARNING MESSAGE IS PRINTED. THIS ALLOWS THE USER TO EXPLICITLY WRITE TEXT INTO A FIXED LINE. ALSO, BY SELECTING A LINE ALREADY PASSED, THE USER CAN BACK UP ON A PAGE AND PRODUCE MULTI-COLUMN PAGES. BOTH OF THESE FEATURES MUST BE USED WITH CARE.

*FIX N,N...

THIS COMMAND PROVIDES THE CAPABILITY OF PROTECTING THE CONTENTS OF A LINE FROM BEING OVERWRITTEN OR CLEARED WHEN A PAGE IS PRINTED. THE CONTENTS OF THE SPECIFIED LINES WILL APPEAR THE SAME ON ALL SUBSEQUENT PAGES WITHIN THE DOCUMENT UNTIL EXPLICITLY CLEARED. (THE INDEXING FEATURE WILL CLEAR ALL FIXED LINES PRIOR TO PRODUCING THE INDEX.) WHEN A LINE NUMBER OF ZERO IS SPECIFIED, ALL NON-BLANK LINES IN THE CURRENT PAGE ARE FIXED. BLANK LINES MUST BE FIXED BY SPECIFYING THEIR LINE NUMBERS DIRECTLY.

*FREE N,N...

THIS COMMAND IS THE INVERSE OF THE *FIX COMMAND IN THAT IT RELEASES AND CLEARS THE LINES SPECIFIED. WHEN A LINE NUMBER OF ZERO IS SPECIFIED, ALL 62 LINES ARE CLEARED AND RELEASED.

*NEED N

THIS COMMAND IS A CONDITIONAL LINE ADVANCE OR PAGE EJECT. IF THERE ARE N CONSECUTIVE UNFIXED LINES FOLLOWING THE CURRENT LINE NO ACTION IS TAKEN. OTHERWISE, THE POINTER IS ADVANCED TO THE FIRST LINE OF A BLOCK OF N UNFIXED LINES OR TO THE START OF A NEW PAGE.

*MARK OFF/ON[,[N],[K]]

THIS COMMAND PROVIDES THE FACILITY FOR MARKING PORTIONS OF A DOCUMENT. THE CHARACTER K IS PLACED IN COLUMN N OF THE LINE(S) WITHOUT AFFECTING TEXT POSITIONING. N MAY BE ANY COLUMN WITHIN THE LEFT MARGIN AND K MAY BE ANY SINGLE CHARACTER. DEFAULTS ARE COLUMN 5 AND THE * CHARACTER. THIS COMMAND MAY BE USED IN TWO MODES, ONE-SHOT OR CONTINUOUS LINE MARKING. WHEN ONLY [N],[K] OR NO PARAMETERS ARE SPECIFIED, ONLY THE CURRENT LINE IS MARKED. WHEN N OR K ARE SPECIFIED THEY BECOME THE NEW DEFAULTS. WHENEVER THE WORD ON IS SPECIFIED, (MUST PRECEED [N,K]), CONTINUOUS MARKING STARTS AND IS ONLY STOPPED WHEN A *MARK OFF COMMAND IS ENCOUNTERED.

*PARA [TEXT]

THIS COMMAND PRODUCES A LINE SKIP EQUAL TO THE *CONTROL PARAMETER AND POSITIONS THE TEXT INDENTED TWO SPACES TO SIGNAL A NEW PARAGRAPH. A PROVISION WAS MADE TO START A NEW PAGE IF LESS THAN TWO LINES OF THE PARAGRAPH CAN BE PRINTED ON THE PAGE.

*DATE
*TIME

THESE TWO COMMANDS INSERT AT THE CURRENT TEXT POSITION AN 8 CHARACTER TEXT STRING CONTAINING THE CURRENT DATE OR TIME IN THE FORM MM/DD/YY OR HH.MM.SS RESPECTIVELY. POSITIONING IS PROVIDED BY PRECEDING COMMANDS.

*PAGE [X],[L],[M,[C]]

WHERE: X = NEW PAGE NUMBER (MIXED)
L = LINE NUMBER (DEFAULT 62)
M = POSITIONING MODE L,C,R (DEFAULT C)
C = COLUMN NUMBER (DEFAULT 44)

THIS COMMAND PRINTS THE CURRENT PAGE IF THERE ARE ANY UNFIXED LINES CONTAINING TEXT AND BEGINS A NEW PAGE. IT ALSO DEFINES THE NEW PAGE NUMBER AND IT'S POSITIONING ON THE PAGE.

THE MIXED NUMBER ENTRY, [X], REPRESENTS THE PAGE NUMBER WHICH WILL BE INCREMENTED BY ONE FOR EACH PAGE UNTIL CHANGED OR TURNED OFF. PAGE NUMBERING MAY BE TURNED OFF BY SPECIFYING A ZERO. WHEN THE PAGE NUMBER IS NOT SPECIFIED, THE PREVIOUS VALUE IS INCREMENTED IF NON-ZERO. THUS A *PAGE COMMAND WITH NO PARAMETERS SIMPLY STARTS A NEW PAGE.

THE REMAINING ENTRIES DEFINE THE POSITIONING OF THE PAGE NUMBER AND REMAIN IN EFFECT UNTIL RESPECIFIED. [L] IS THE LINE NUMBER WITH AN INITIAL DEFAULT OF 62 (LAST LINE). [M] IS A SINGLE CHARACTER WHICH DEFINES THE METHOD OF POSITIONING ON THE LINE WITH REFERENCE TO THE COLUMN NUMBER [C]. [M] MUST BE L, C, OR R FOR LEFT JUSTIFIED, CENTERED, OR RIGHT JUSTIFIED RESPECTIVELY. WHEN [C] IS UNSPECIFIED THE DEFAULT TAKEN IS BASED ON THE CURRENT MARGIN VALUES. THUS, [M] AND [C] ARE LINKED TOGETHER AND [M] ALWAYS CAUSES [C] TO BE REDEFINED.

THE LINE WHERE THE PAGE NUMBER APPEARS IS AUTOMATICALLY PROTECTED (FIXED) WHEN THE PAGE NUMBER IS NON-ZERO. WHENEVER THE POSITIONING OF THE PAGE NUMBER CHANGES, THE LINE PREVIOUSLY SELECTED IS CLEARED (FREED) AND THE NEW LINE IS FIXED. THIS COULD RESULT IN LOSS OF TEXT ELSEWHERE IN THE OLD LINE.

INDEXING FEATURE

*KEY <ENTRY> [,<ENTRY>...]
<ENTRY> ::= <LEVEL1>[/<LEVEL2>...../<LEVEL4>]

THIS COMMAND PROVIDES A MEANS FOR DEVELOPING AN INDEX TO A MULTI-PAGE DOCUMENT. THE *KEY COMMANDS ARE INCLUDED WITH THE INPUT TEXT WHERE THE REFERENCE TO THE INDEX ENTRY OCCURS. THESE *KEY COMMANDS DO NOT AFFECT TEXT CONTENT OR PLACEMENT AND APPEAR ONLY ON THE DIAGNOSTIC OUTPUT. EACH ENTRY APPEARS IN THE INDEX WITH THE PAGE NUMBERS WHERE THE ENTRY WAS ENCOUNTERED IN A *KEY COMMAND. WHILE PROCESSING THE TEXT, TYPIST WILL STORE THE INDEX ENTRIES AND PAGE NUMBERS FOR PRODUCTION OF THE INDEX AT THE END OF A DOCUMENT.

THE INDEX ENTRIES MAY BE TREE-STRUCTURED INTO AS MANY AS FOUR LEVELS. THIS STRUCTURE IS REFLECTED BY INDENTING EACH SUB-ENTRY TWO SPACES FROM THE HIGHER LEVEL ENTRY ABOVE IT. IN THIS WAY THE RELATIONSHIPS BETWEEN ENTRIES IS IMPLIED. THE NATURE OF THIS TREE-STRUCTURE REQUIRES THAT EACH OCCURENCE OF A LOWER LEVEL ENTRY MUST BE PRECEEDED BY IT'S ENTIRE

CHAIN OF HIGHER LEVEL ENTRIES SEPARATED BY SLASHES. THE TREE-STRUCTURE IS BUILT WITH ENTRIES IN ALPHABETIC ORDER WITHIN EACH LEVEL. AN EXAMPLE OF THIS STRUCTURING OF ENTRIES IS:

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---COMMANDS---                ---INDEX---
*KEY LVL1/LVL2/LVL3        LVL1
*KEY LVL1/ADDED KEY          ADDED KEY
*KEY LVL1/LVL2/NEXT          LVL2
*KEY OTHER ENTRY               LVL3
                               NEXT
                            OTHER ENTRY
```

THE PAGE NUMBERS WHERE AN ENTRY IS REFERENCED ARE PRINTED IN ORDER OF OCCURENCE AFTER THE ENTRY. SHOULD THE LINE OVERFLOW, THE EXCESS WILL CONTINUE ON THE NEXT LINE INDENTED TWO MORE SPACES.

WHEN THE INDEX IS PRINTED, ALL LINES ARE CLEARED AND THE LAST MARGIN SETTINGS AND PAGE NUMBER POSITIONING ARE USED. IF THE SPACE BETWEEN THE MARGINS IS TWICE THE LENGTH OF THE LONGEST INDEX ENTRY PLUS IT'S INDENTATION, TWO COLUMNS OF INDEX ENTRIES ARE PRINTED ON EACH PAGE. THE FIRST PAGE OF THE INDEX HAS A HEADING AND PAGE NUMBERING CONTINUES AS PART OF THE DOCUMENT.

THE USE OF THIS FEATURE WILL INCREASE THE CORE STORAGE REQUIREMENTS SLIGHTLY ACCORDING TO THE NUMBER AND LENGTH OF UNIQUE INDEX ENTRIES. THE FIELD LENGTH USED IS DISPLAYED IN A DAYFILE MESSAGE FOR EACH DOCUMENT SO THAT ACCURATE ESTIMATES OF FUTURE RUNS CAN BE MADE.

SELECTIVE DOCUMENT PROCESSING

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*DOC NAME
*OPTION NAME,NAME...
*ON NAME,NAME...
*OFF NAME,NAME...
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THESE COMMANDS, IN CONJUNCTION WITH THE O=OPTION PARAMETERS IN THE PROGRAM CALL, PROVIDE A MEANS OF SELECTIVELY PROCESSING OR SKIPPING OVER PORTIONS OF THE INPUT FILE.

A *OPTION COMMAND SIGNALS THE START OF A PORTION OF INPUT TEXT AND/OR COMMANDS WHICH IS TO BE PROCESSED ACCORDING TO A SET OF OPTION NAMES. WHEN AT LEAST ONE NAME IS IN THE LIST OF OPTIONS AND A *OPTION COMMAND IS ENCOUNTERED, THE NAMES ON IT ARE CHECKED AGAINST THE OPTION LIST, AND IF NONE MATCH, SKIPPING IS INITIATED UNTIL ANOTHER *OPTION COMMAND IS FOUND.

THE *DOC COMMAND IS IDENTICAL TO THE *OPTION COMMAND EXCEPT THAT IT ALSO SIGNALS THE START OF A DOCUMENT AND THE FIRST NAME IS THE DOCUMENT NAME WHICH APPEARS IN THE DAYFILE MESSAGE AT THE END OF EACH DOCUMENT. BEFORE STARTING A DOCUMENT, ANY PRECEEDING DOCUMENT IS COMPLETED AND ALL DEFAULTS EXCEPT THE OPTION LIST ARE RESET ACCORDING TO THE PROGRAM CALL.

THE *ON AND *OFF COMMANDS TURN ON AND OFF OPTION NAMES WHEN ENCOUNTERED WITHIN THE INPUT. THEY ARE SUBJECT TO BEING SKIPPED OVER ACCORDING TO THE STRUCTURE OF *OPTION AND *DOC COMMANDS AND CONSEQUENTLY PROVIDE A LIMITED LOGIC CAPABILITY IN THE PROCESSING OF TEXT. FOR EXAMPLE, ONE OPTION CAN BE USED TO TURN ON SEVERAL OR TO TURN OFF OTHERS INCLUDING ITSELF (ONCE-ONLY SWITCH).

THERE ARE MANY PRACTICAL USES OF THESE COMMANDS TO MANIPULATE TEXT AND DOCUMENTS. ONE USE IS IN DEVELOPING A PARAMETERIZED DISTRIBUTION LIST FOR REPORTS, MEMOS, AND NOTICES WITH VARIABLE NUMBERS OF COPIES DEPENDING UPON THE NAMES (OF PEOPLE) TURNED ON BY A SINGLE OPTION. ANOTHER USE IS IN A LIBRARY OF PROGRAM DOCUMENTATION WHICH CAN BE ACCESSED BY DOCUMENT NAME OR SUBJECT (OPTIONS).

OVER-PRINTING CONTROL

*BOLD [N],[TEXT]

THIS COMMAND ALLOWS CONTROL OF THE AMOUNT OF REPEATED PRINTING OF PORTIONS OF THE TEXT, AND REMAINS IN EFFECT UNTIL CHANGED BY A NEW *BOLD COMMAND.

THE NUMBER N MAY BE ABSENT, 0, OR RANGE FROM 1 TO 7. IF N IS ABSENT, THE AMOUNT OF OVER-PRINTING IS INCREASED BY 1. (AN ATTEMPT TO GO OVER 7 IS DIAGNOSED AS AN ERROR.) IF N IS ZERO, THE AMOUNT OF OVER-PRINTING REVERTS TO THE LAST NON-ZERO VALUE SPECIFIED. IF N IS 1, THE TEXT WILL BE PRINTED ONCE. IF N IS 7, THE TEXT WILL BE PRINTED 7 TIMES. IF ↑ IS USED TO OVER-PRINT AS WELL, THE SUM (NOT THE PRODUCT) OF THE PRINT COUNTS IS USED.

TABLE 1 - TYPIST COMMANDS

PARAMETERS:

ABV	SYNTAX	DEFAULT	EXPLANATION
*SZ	*SIZE N	80	INPUT LINE LENGTH
*LM	*LIMIT N	80	OUTPUT LINE LIMIT
*CP	*COPY N	1	NUMBER OF COPIES DESIRED
*RP	*REPEAT	1	REPEAT PAGES N TIMES
*CL	*CONTROL N	1	SET LINE SPACING.
*MR	*MARGINS N,N	9,80	SET REFERENCE/WORKING MARGINS
*IN	*INDENT [N],[N]	0,0	MOVE WORKING MARGINS INWARD
*TS	*TABS N1,N2...,N20	-	DEFINE TAB POSITIONS.

TEXT FORMATING COMMANDS:

*TB	*TAB [N],[TEXT]	NEXT	MOVE TO TAB POSITION
*CR	*CENTER [N],TEXT	MRGS/2	CENTER TEXT ABOUT A COLUMN
*RT	*RIGHT [N],TEXT	R.MRG	RIGHT JUSTIFY TEXT TO A COLUMN
*LF	*LEFT [N],[TEXT]	L.MRG	LEFT JUSTIFY TEXT TO COLUMN N
*SP	*SPACE [N],[TEXT]	1	SPACE OVER N SPACES
*SK	*SKIP [N],[TEXT]	0	SKIP DOWN N*CONTROL LINES
*LN	*LINE [N],[TEXT]	NEXT	SKIP DOWN TO LINE N
*FX	*FIX N,N,...	-	PROTECT LINE CONTENTS
*FR	*FREE N,N,...	-	RELEASE AND CLEAR LINES
*ND	*NEED N	1	CONDITIONAL NEW PAGE
*PR	*PARA [TEXT]	-	SKIP A LINE AND INDENT TEXT
*PG	*PAGE [X],[L],[M,[G]]	NEXT	DEFINE NEW PAGE AND NUMBERING
*PK	*PACK ON/OFF	ON	START OR STOP TEXT COMPACTING

SELECTIVE PROCESSING COMMANDS:

*DO	*DOC NAME	-	RESET DEFAULTS AND START NEW DOCUMENT
*OP	*OPTION NAME,NAME...	-	PROCESS TEXT IF A NAMED OPTION IS ON
*ON	*ON NAME,NAME...	-	TURN ON NAMED OPTIONS
*OF	*OFF NAME,NAME...	-	TURN OFF NAMED OPTIONS

MISCELLEANOUS COMMANDS:

*DT	*DATE	-	PROVIDE DATE IN FORM MM/DD/YY
*TM	*TIME	-	PROVIDE TIME IN FORM HH.MM.SS
*MK	*MARK OFF/ON[,[N],[K]]	5,*	MARK LINE(S) WITH K IN COL. N
*KY	*KEY ENTRY,ENTRY...	-	STORE INDEX ENTRIES
*BO	*BOLD [N],[TEXT]	1	SET REPEATED PRINT COUNT

WHERE:

[] = OPTIONAL ENTRY
/ = CHOICE OF ENTRIES
N = AN UNSIGNED NUMBER
X = MIXED NUMBER (LAST CHAR. MUST BE DIGIT)
K = SINGLE NON-BLANK CHARACTER
NAME = SINGLE WORD OF UP TO 8 CHAR.
ENTRY = STRUCTURED INDEX ENTRY PHRASE
TEXT = FREE-FORM TEXT (LEADING/TRAILING BLANKS IGNORED)

I N D E X

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VECTOR IS A LIBRARY OF 3-SPACE MANIPULATION ROUTINES. MOST COMMON VECTOR OPERATIONS ARE SIMULATED IN THE PACKAGE. IT IS REQUIRED THAT EACH INPUT VECTOR BE STORED IN THREE SEQUENTIAL LOCATIONS (ONLY THE STARTING POINT IS USED IN THE ROUTINE CALLS). EACH INPUT MATRIX MUST BE STORED ROW BY ROW IN NINE SEQUENTIAL LOCATIONS. NOTE THAT THE SUBROUTINE VEC MAY BE USED TO ASSEMBLE ANY THREE DATA INTO A VECTOR (OR A MATRIX-S ROW). IN GENERAL, IT IS NOT SAFE TO INDISCRIMINATELY STORE VECTORS INTO THEMSELVES. CARTESIAN COORDINATES ARE ASSUMED THROUGHOUT.
IN THE FOLLOWING TABLE THE FOLLOWING CONVENTIONS WILL BE USED--

A,B,C = VARIABLE NAMES FOR MATRICES

W,X,Y,Z = VARIABLE NAMES FOR VECTORS

F,G,H = VARIABLE NAMES FOR SCALARS

SUBROUTINE OR FUNCTION NAME	CALL	USE
DOT	F = DOT(X,Y)	COMPUTE THE DOT PRODUCT OF TWO VECTORS
CROSS	CALL CROSS(X,Y,Z)	Z = X CROSS Y
UNIT	CALL UNIT(X,Y)	RETURN Y EQUAL TO THE DIRECTION COSINES OF X
AMAG	F = AMAG(X)	RETURN F EQUAL TO THE MAGNITUDE OF X
VECSUM	CALL VECSUM(X,Y,Z)	Z = X + Y
VECDIF	CALL VECDIF(X,Y,Z)	Z = X - Y
CONMUL	CALL CONMUL(X,F,Y)	Y = F * X
VECMUL	CALL VECMUL(X,A,Y)	Y = A * X
MATMUL	CALL MATMUL(A,B,C)	C = A * B
VEC	CALL VEC(X,F,G,H)	COMPOSE A VECTOR X FROM THREE SCALARS F,G,H
UNVEC	CALL UNVEC(X,F,G,H)	SET THREE SCALARS EQUAL TO COMPONENTS OF A VECTOR X
CPYVEC	CALL CPYVEC (X,Y)	Y = X (I.E. COPY X INTO Y)
CPYMAT	CALL CPYMAT(A,B)	COPY MATRIX A INTO MATRIX B
ALNGTH	F = ALNGTH(X,Y)	RETURN THE DISTANCE BETWEEN THE ENDS OF TWO VECTORS
ANGLE	F = ANGLE(X,Y,Z)	RETURN THE ANGLE (IN DEGREES) BETWEEN THE VECTORS Y TO X AND Y TO Z
TORSIN	F = TORSIN(W,X,Y,Z)	RETURN THE DIHEDRAL ANGLE (IN DEGREES) BETWEEN THE PLANES W,X,Y AND X,Y,Z THE ANGLE RETURNED WILL HAVE A VALUE APPROPRIATE FOR A RIGHT-HANDED ROTATION ABOUT THE LINE FROM X TO Y
INVER	CALL INVER(A,B)	RETURN MATRIX B EQUAL TO THE INVERSE OF MATRIX A
TRNSPZ	CALL TRNSPZ(A,B)	RETURN MATRIX B EQUAL TO THE TRANSPOSE OF MATRIX A
CART	CALL CART(CELL,A)	RETURN A MATRIX (A) WHICH CONVERTS INPUT CELL COORDINATES TO CARTESIAN COORDINATES (CELL MUST BE THE THREE CELL LENGTHS AND THE INTERAXIAL ANGLES OR COSINES IN SEQUENTIAL STORAGE). IF THE RECIPROCAL CELL IS INPUT AND REAL COORDINATES ARE DESIRED, THE RESULTING MATRIX WILL BE THE INVERSE-TRANSPOSE OF THE DESIRED ONE. THE DETERMINANT OF A IS THE VOLUME OF THE INPUT CELL. (I.E. THE RECIPROCAL CELL VOLUME IF THE RECIPROCAL CELL WAS INPUT.)

DET	F = DET(A)	RETURNS THE VALUE OF THE DETERMINANT OF A MATRIX. (THIS IS THE CELL VOLUME IF THIS IS AN ORTHOGONALIZING MATRIX).
ROTMAT	CALL ROTMAT (X,F,A)	PRODUCE A MATRIX FOR THE ROTATION ABOUT A VECTOR (X) BY AN ANGLE (F, IN RADIANS)
GENROT	CALL GENROT(X,Y,F,A,Z)	FOR ROTATION ABOUT THE LINE BETWEEN X AND Y BY AN ANGLE (F, IN RADIANS), GENROT RETURNS A ROTATION MATRIX AND A DISPLACEMENT VECTOR Z
UNITRY	CALL UNITRY(A,B)	B IS RETURNED AS THE GRAM-SCHMIDT ORTHOGONALIZATION OF A
EIGEN1	F = EIGEN1(A,X,B)	FOR AN INPUT MATRIX (A) EIGEN1 RETURNS THE VALUE OF THE EIGENVALUE WITH THE LARGEST ABSOLUTE VALUE. X IS RETURNED AS THE CORRESPONDING EIGENVECTOR. B IS THE -DEFLATED- MATRIX, WHICH MAY BE EXAMINED FOR EQUAL EIGENVALUES.
INRTIA	CALL INRTIA (X,F,A)	SUMS UP THE APPROPRIATE ELEMENTS OF THE INERTIA TENSOR (A) FOR THE END POINTS OF A LIST OF VECTORS (X) WITH WEIGHTS (F). THIS ROUTINE MUST BE CALLED ONCE FOR EACH VECTOR, AND -A- MUST BE ZEROED BY THE USER AT THE BEGINNING OF EACH NEW TENSOR. IF AN INERTIA TENSOR IS CALCULATED FOR A GROUP OF POINTS, AND THE CENTER OF MASS IS USED AS THE ORIGIN, THEN THE EIGENVECTOR OF THE LARGEST EIGENVALUE IS NORMAL TO THE BEST PLANE THROUGH THE POINTS, AND THE EIGENVECTOR OF THE LARGEST EIGENVALUE OF THE INVERSE MATRIX IS THE BEST LINE.
ACOS	F = ACOS (G) F = ARCOS(G)	RETURNS F AS THE ANGLE (IN RADIANS) WHICH HAS G AS ITS COSINE
ASIN	F = ASIN (G) F = ARSIN(G)	RETURNS F AS THE ANGLE (IN RADIANS) WHICH HAS G AS ITS SINE
MAT	CALL MAT(A,X,Y,Z)	STORE THREE VECTORS (AS ROWS) INTO A MATRIX
SOLVE	CALL SOLVE (S,T,U,V)	ACCEPT 3 PLANES STORED AS VECTORS PLUS ONE WORD FOR THE CONSTANT AND RETURN V AS THE VECTOR TO THE POINT OF INTERSECTION (EACH PLANE MUST BE FOUR ADJACENT WORDS IN CORE)
UNMAT	CALL UNMAT(A,X,Y,Z)	CONVERT THE ROWS OF A MATRIX INTO VECTORS
PAIR	CALL PAIR(W,X,Y,Z,A)	MATRIX A IS RETURNED AS THE ROTATION MATRIX WHICH MAKES W PARALLEL TO Y AND X AS CLOSE TO PARALLEL TO Z AS POSSIBLE GIVEN THE FIRST CONSTRAINT
PAIRSM	CALL PAIRSM (X,Y,A,B)	WITH THE HELP OF SUBROUTINE PAIREN, GET THE MATRIX WHICH GIVES THE BEST LEAST-SQUARES FIT OF X TO Y--THAT IS IF THE X-S ARE MULTIPLIED BY THE FINAL MATRIX FROM PAIREN THE BEST FIT RESULTS. CALLED REPEATEDLY, FOLLOWED BY ONE CALL TO PAIREN
PAIREN	CALL PAIREN (A,B,C)	FINISHES CALCULATION OF BEST FIT TENSOR (C) USING SUMS FROM PAIRSM--NOTE THAT C TIMES C TRANSPOSE IS THE METRIC TENSOR WHICH RELATES THE TWO SETS OF VECTORS

******AUXILARY ROUTINES WHICH MAY NOT BE TRANSPORTABLE*****

INSYM	J=INSYM(ALIN,N,A,X)	THE REAL ARRAY ALIN IS INPUT AS A1 VARIABLES (N OF THEM) AND A AND X ARE THE DECODED SYMMETRY ELEMENT WHICH WERE INPUT IN THE FORM X,1/2-Z,1/3-Z+X J = 0 NO ERRORS J = 1 ILLEGAL CHARACTER FOUND J = 2 NON-UNITARY MATRIX OR A TRANSLATION NOT POSSIBLE IN A SPACE GROUP

THE ROW ORDER IN WHICH MATRICES ARE STORED FOR VECTOR WAS CHOSEN BECAUSE IT RESULTS IN SIMPLER CODING. HOWEVER, IT

CONFLICTS WITH THE ORDER THAT DOUBLY SUBSCRIPTED FORTRAN VARIABLES ARE LAID OUT. THE ORDER CAN BE CONVERTED BY A CALL TO TRNSPZ. E.G.--IF A IS A MATRIX IN COLUMN ORDER:

```
DIMENSION A(3,3), B(9)
---------
CALL TRNSPZ (A,B)
```

WILL RESULT IN A MATRIX B WHICH CAN BE USED BY VECTOR. TWO WAYS OF STORING INFORMATION FOR VECTOR SUGGEST THEMSELVES--VARIABLES CAN BE LAID OUT IN LONG ARRAYS WITH A SINGLE SUBSCRIPT, OR IF DOUBLE SUBSCRIPTS ARE USED, IT IS CONVENIENT TO MAKE 100 VECTORS BY -- DIMENSION X(3,100) , AND 100 MATRICES BY -- DIMENSION A(9,100)

VECTOR MAY BE INSTALLED BY COMPILING UNDER FORTRAN AND MAKING A LIBRARY (E.G. VECTOR.OBJ) WHICH MAY BE USED IN LINKING. ALL VARIABLES USED AS CALLING PARAMETERS ARE FLOATING POINT SO THAT NO CONFLICTS IN WORD LENGTH SHOULD ARISE. I BELIEVE THAT NO MACHINE DEPENDENT CODE IS INCLUDED SO THE CODE SHOULD BE TRANSPORTABLE. A COMMON /VECCOM/ IS USED TO REDUCE THE AMOUNT OF STORAGE REQUIRED, BUT IT IS NOT USED TO TRANSMIT DATA AND MAY BE REPLACED SAFELY BY APPROPRIATE DIMENSION STATEMENTS.

LIBRARY AND WRITEUP WRITTEN AT BROOKHAVEN NATIONAL LABORATORY, SPRING AND SUMMER, 1974 BY LARRY ANDREWS, CRYSNET PROJECT
*****RELEASED ONLY AS A PREPRINT*****

VECTR1 IS A CALLING PACKAGE FOR THE SUBROUTINE PACKAGE VECTOR. THE BASIC PURPOSE IS TO EMULATE THE OPERATION OF THE HEWLITT-PACKARD HAND-HELD CALCULATORS. SEPARATE STACKS ARE PROVIDED FOR CONSTANTS, VECTORS, AND MATRICES. EACH MAY BE ACCESSED SEPARATEL AND THEY MAY BE USED TOGETHER TO FORM MORE COMPLEX OPERATIONS. THREE BASIC FUNCTIONS ARE PROVIDED: DATA INPUT, MANIPULATIVE INSTRUCTIONS, AND OPERATIONS FOR DOING CALCULATIONS. ALL ANGLES ARE ASSUMED TO BE INPUT AND RETURNED IN DEGREES.

FIRST WE WILL CONSIDER DATA INPUT. FOUR PREFIXES ARE PROVIDED: C,V,M, AND " " (THAT'S A BLANK). A NUMBER PRECEEDED BY C WILL BE INTERPRETED AS SCALAR (CONSTANT) AND PUT INTO THE SCALAR STACK, WHICH WILL BE PUSHED DOWN. A TRIPLE OF NUMBERS PRECEEDED BY V WILL BE INTERPRETED AS A VECTOR AND PUT INTO THE VECTOR STACK, WHICH WILL BE PUSHED DOWN. SIMILARLY, M PRECEEDS NINE NUMBERS REPRESENTING A MATRIX (IN ROW ORDER). A BLANK PRECEEDING AN INPUT WILL BE TAKEN TO MEAN THAT THE INPUT IS OF THE SAME TYPE AS THE PRECEEDING INPUT. IF A LINE BEGINS WITH A NUMBER, THE ENTRY IS ASSUMED TO BE THE SAME TYPE AS THE LAST DATA INPUT.

THE MANIPULATION INSTRUCTIONS ARE: P,S,R,X,E, AND U. THEY EACH MUST BE FOLLOWED IMMEDIATELY BY ONE OF THE DATA-INPUT CODES, AS SUFFIXES (C,V,M, OR " ", WHERE BLANK IS USED TO MEAN ALL THREE). THE FUNCTIONS ARE:

P	PRINT
S	SAVE (STORE IN A MEMORY FOR THE APPROPRIATE DATUM)
R	ROLL THE APPROPRIATE STACK ONE ELEMENT
X	EXCHANGE THE UPPERMOST TWO ELEMENTS OF THE DESIGNATED STACK
E	ENTER THE LAST-INPUT QUANTITY OF THE DESIGNATED TYPE AGAIN
U	UNSAVE (TAKE A STORED QUANTITY AND PUT IT ONTO A STACK)
Z	ZERO THE TOP ENTRY OF THE DESIGNATED STACK, WITHOUT SHIFTING THE OTHER ELEMENTS
W	WRITE TO UNIT 1 THE APPROPRIATE ELEMENTS (FORMAT IS 1X,3F10.4)

FOR EACH OF THE INSTRUCTIONS THERE ARE FOUR POSSIBLE USES; FOR INSTANCE, FOR P WE CAN HAVE PC,PV,PM, AND P MEANING: PRINT THE TOP CONSTANT,THE TOP VECTOR ,THE TOP MATRIX, OR THE TOP ELEMENT OF EACH TYPE. IN ADDITION, E HAS THE OPTION OF BEING FOLLOWED BY A DIGIT, N, (=1 TO 5) WHICH SPECIFIES THAT THE TOP N ELEMENTS OF THE SPECIFIED TYPE ARE TO BE REENTERED IN THE SAME ORDER.

THE CALCULATION CODES WILL REMOVE ANY QUANTITIES USED IN THE CALCULATIONS FROM THE STACKS AND PUSH IN ANY CALCULATED QUANTITIES. FOR EXAMPLE, DOT WILL REMOVE TWO VECTORS AND PUSH DOWN ONE NEW SCALAR. ALL OPERATIONS ARE IN REVERSE POLISH ALGORITHM: THAT IS THE FIRST QUANTITIES TO BE USED IN A CALCULATION ARE INPUT FIRST AND IF THE OPERATION PERFORMED IS ORDER-DEPENDENT, THE LAST OPERATOR OF SOME TYPE WILL BE THE LAST ONE INPUT TO ITS STACK. THE CODES FOR USE WITH VECTORS AND MATRICES AR

DOT	CALCULATE A DOT PRODUCT FROM THE LAST TWO INPUT VECTORS
CRS	CALCULATE A CROSS PRODUCT FROM THE LAST TWO INPUT VECTORS
SUM	CALCULATE THE SUM OF THE LAST TWO VECTORS
DIF	CALCULATE THE VECTOR DIFFERENCE OF THE LAST TWO VECTOR (THE NEXT TO LAST MINUS THE LAST)
EIGN	GET THE EIGENVALUE WITH LARGEST ABSOLUTE MAGNITUDE AND ITS EIGENVECTOR (USING LAST INPUT MATRIX)
MAG	CALCULATE THE MODULUS OF THE TOP VECTOR
UNIT	CONVERT THE TOP VECTOR TO A UNIT VECTOR
CV	MULTIPLY THE TOP VECTOR BY THE TOP CONSTANT
VC	SAME AS CV
MV	PREMULTIPLY THE TOP VECTOR BY THE TOP MATRIX
MM	MULTIPLY THE THE TOP TWO MATRICES (THE LAST INPUT MATRIX BEING THE POST-MULTIPLIER)
TRNZ	CALCULATE THE TRANSPOSE OF THE TOP MATRIX
INV	CALCULATE THE INVERSE OF THE TOP MATRIX
DET	CALCULATE THE VALUE OF THE DETERMINANT OF THE TOP MATRIX
UNTR	CALCULATE A UNITARY MATRIX BY GRAM-SCHMIDT ORTHOGONALIZATION OF THE TOP MATRIX
INRT	USE THE TOP VECTOR TO SUM INTO AN INERTIA TENSOR. THE INERTIA TENSOR IS STORED IN THE TOP OF THE MATRIX STACK WHICH SHOULD BE ZEROED BEFORE STARTING THIS CALCULATION
LNGT	GET THE DISTANCE BETWEEN THE ENDS OF THE TWO TOP VECTORS
ANGL	GET THE ANGLE (IN DEGREES) BETWEEN THE ENDS OF THE TOP THREE VECTORS (THE CENTRAL VECTOR IS THE SECOND ONE INPUT)
TRSN	GET THE TORSION ANGLE (IN DEGREES) BETWEEN THE ENDS OF THE TOP FOUR VECTORS. THE ANGLE IS RETURNED ASSUMING THAT THE SENSE IS MEANT TO BE RIGHT-HANDED FROM THE TOPMOST VECTOR IN A CONTINUOUS STRING TO THE FOURTH FROM THE TOP (THE REVERSE ORDER GIVES THE SAME VALUE)
CAPT	GET THE MATRIX TO CONVERT TO A CARTESIAN SYSTEM ASSUMING THAT THE TOP VECTOR IS THE LENGTHS OF THE SIDES OF THE UNIT CELL AND THE NEXT VECTOR IS THE INTERAXIAL ANGLES OR THEIR COSINES
ROT1	GET THE MATRIX FOR ROTATION ABOUT THE TOP VECTOR BY THE TOP CONSTANT

CODES PROVIDED FOR MANIPULATION OF SCALARS ONLY ARE:

ASIN	ARC SINE
ACOS	ARC COSINE
ATAN	ARC TANGENT
X**Y	X (SECOND ELEMENT OF STACK) TO THE POWER OF Y (TOP OF STACK)
SQRT	SQUARE ROOT
SIN	SIN

COS	COSINE
TAN	TANGENT
LOG	BASE 10 LOGARITHM
LN	BASE E LOGARITHM
EXP	EXPONENTIAL
1/X	RECIPROCAL
PI	3.1415927
RD	CONVERT FROM RADIANS TO DEGREES
DR	CONVERT FROM DEGREES TO RADIANS
*	MULTIPLY
+	ADD
-	SUBTRACT
/	DIVIDE

THERE ARE ALSO TWO PROGRAM FUNCTIONS:

STAK	CHANGE THE STACK HEIGHT: THE INITIAL VALUE IS 4: THE MAXIMUM VALUE IS 10. VALUE IS TAKEN FROM STACK.
LABL	SWITCH TO ECHO COMMAND LABELS TYPED IN. TYPING LABL AT ANY TIME WILL REVERSE THE CURRENT EFFECT. INITIAL VALUE IS FOR NO ECHO

AUTHOR: H.J.BERNSTEIN

WEEKEND - 03/10/76

BROOKHAVEN NATIONAL LABORATORY
CHEMISTRY DEPARTMENT

CRYSNET PROGRAM WRITEUP

CDC CYBER 70/74,CDC CYBER 70/76
CDC SCOPE 3.4, CDC SCOPE 2.1

PURPOSE

WEEKEND IS A PROGRAM TO DETERMINE IF THE DAY OF EXECUTION IS ON THE WEEKEND.

INTRODUCTION

IN ORDER TO TAKE ADVANTAGE OF CHEAPER WEEKEND RATES, A JOB MUST START IN EXECUTION BETWEEN 6 PM ON FRIDAY, AND 9 AM ON MONDAY. FOR A VERY LARGE JOB, THE DIFFERENCE IN COST BETWEEN WEEKEND, AND NON-WEEKEND RUNNING MAY BE SO LARGE, THAT THE USER DOES NOT WISH THE JOB TO RUN AT ALL, IF IT STARTS EXECUTION OUTSIDE OF THIS PERIOD. THE PROGRAM WEEKEND WILL ABORT IF EXECUTED OUTSIDE THIS PERIOD.

USE

ONCE ATTACHED (USUALLY VIA ACCESS) WEEKEND IS EXECUTED BY

```
WEEKEND.
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WHICH WILL CAUSE A JOB ABORT IF THE DAY AND TIME OF EXECUTION DO NOT FALL WITHIN THE PERIOD 1800 FRIDAY TO 0859 MONDAY.

MESSAGES

WEEKEND MAY ISSUE EITHER ONE OR TWO MESSAGES:

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UTCWEA- TODAY IS XXXXXXX
UTCWEB- NOT THE WEEKEND - ABORT
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THE FIRST MESSAGE IS ALWAYS ISSUED, WITH "XXXXXX" REPLACED BY THE DAY OF EXECUTION (MONDAY,TUESDAY, ETC.) THE SECOND MESSAGE IS ISSUED ONLY IF WEEKEND IS RUN DURING THE WEEK.

NAME: XDATA | AUTHOR(s): F. Bernstein

CORE: 30K (40K if RUN is used) | DATE: November 1973

```
PROGRAM XDATA(DATA,FØUR,INPUT,ØUTPUT,PUNCH,TAPE18,TAPE3,TAPE15=DATA,
      TAPE19=FØUR,TAPE5=INPUT,TAPE6=ØUTPUT)
```

I. PURPOSE:

To obtain scale and temperature factors using Wilson plot.

II. TAPES:

A. DATA- binary data tape	Format - ISENT,H1,H2,H3,FSQ,SIG, SCALEN,E1
B. TAPE18- least squares binary output	Format - ISENT,H1,H2,H3,FSQ,FSCALEN,E1
C. FØUR	Format - IH,IK,IL,SINTHL,ØRD,SHARP,COSWH, SINWH,SHNOO

III. LIMITATIONS:

NF - number of form factor tables	10
NY - points in Wilson plot	15
NSCALE - number of scale factors	20

IV. REPLACEABLE SUBROUTINES:

A. IMP

B. WEIGHT

V. DECK SET UP

A. JOB CARD

1. TIME LIMIT - ?
2. FIELD LENGTH - 30-40 K
3. NUMBER OF TAPES - 0-3
4. ECS - none

B. CONTROL CARDS

```
ATTACH(XDATA,XDATA,ID=CPRØGS)
FTN(SYSEDIT) } if subroutines
LØAD(LGØ)    }
REQUEST etc. of tapes
XDATA.
```

C. DATA CARDS:

CARD	FORMAT
Title	8A6
Control integers	24I3
Form factor tables	8F9.3
NA	24I3
SINMAX	F9.3
Reciprocal cell constants	6F9.3
Optional-format statement	12A6
Data cards	I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3,F5.1

D. REMOTE FILES:

ØUTPUT

Brookhaven Crystallographic Computer Program

NAME: XDATA FILES: 8 TIME: less than 1 minute for most applications

FL: 30K (50K if FTN is used)

Purpose: To obtain scale factors and overall temperature factors from Wilson plots, to put out scaled data on tape suitable for input to CLINUS, and to put out data on tape for input to JIMDAP to calculate either ordinary Patterson, sharpened Patterson, or sharpened Patterson with origin removed.

Note that XDATA does not properly take account of multiplicities when incomplete data sets are used. This is a minor perturbation for three-dimensional data. If all unobserved reflections (including space group extinctions) are included, the multiplier $S/\sum$ as defined by Rogers is unity for all classes of reflections, so no special handling is necessary.

PRØGRAM XDATA(DATA,FØUR,INPUT,ØUTPUT,PUNCH,TAPE18,TAPE3,TAPE15=DATA, TAPE19=FØUR,TAPE5=INPUT,TAPE6=ØUTPUT)

Data Input:

1. TITLE FØRMAT(8A6)

2. FØRMAT(24I3) IC(I), I = 1,24 Control integers.

   IC(1) = NF = number of different form factor tables.

   IC(2) = NX = number of points to be used in Wilson plot. Maximum 15.

   IC(3) = NSCALE = number of scale factors to be determined from Wilson plot.

   IC(4) = 1 if reflection data is on cards.

   = 2 if reflection data is to be read in variable Format and IMP is called.

   = 3 if reflection data is on binary tape.

   IC(5) = 0 if no output desired for least squares

   = 1 if new cards are to be punched for least squares

   = 3 if binary tape to be written for least squares

   IC(6) = 0 if no output for Patterson

   = 1 if binary tape is to be written for Patterson

   IC(7) = 1 suppress printed output of CLINUS and JIMDAP data cards or tapes

   IC(8) $\neq$ 0 read F

   = 0 read F^2

3. FØRMAT(8F9.3) Form factor tables as for CLINUS. NF tables, four cards per table:

Card						
	i.	form	factors	for	SINTHL	= 0.00(0.05) 0.35
	ii.	"	"	"	"	= 0.40(0.05) 0.75
	iii.	"	"	"	"	= 0.80(0.05) 1.15
	iv.	"	"	"	"	= 1.20(0.05) 1.55

4. FØRMAT(24I3) NA(I), I = 1, NF. The number of atoms in the unit cell of each form factor type.

5. FØRMAT(F9.3) SINMAX, the maximum value of $\sin\theta/\lambda$ to be considered in Wilson plot. All data will be corrected.

6. FØRMAT(6F9.3) Reciprocal cell constants, a*,b*,c*,cosalpha*, cosbeta*,cosgamma*.

7. OPTIONAL. SUPPLY ONLY IF IC(4) = 2. FØRMAT(12A6)
   Variable FØRMAT statement (DATFØR(I),I=1,12) must start and end with parentheses.

8. Reflection cards if supplied. (If IC(4)=2, FØRMAT will be that specified on optional card 7.)
   FØRMAT(I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3,F5.1) ISENT,h,k,ℓ,F^2,$\sigma(F^2)$, scale factor number, E1(I), I=1,8
   ISENT = 0 terminated by ISENT=1 and remainder of card blank
   E1 = extra floating point input DIMENSION E1(25)
   E2 = extra floating point input
   If IC(8)$\neq$0 then actually read F rather than F^2

Input Data Tapes:

If Binary data tape is called for, the file to be used is DATA and the record is read as follows:

```
READ (15), ISENT,H1,H2,H3,FSQ,SIG,SCALEN,E1
```

Dimensions:

The program as compiled allows the following maximum values.

NF = 10

NX = 15

NSCALE = 20

Number of reflections unlimited.

Output

The first reflection listed in all the output will be (000). $F^2(000)$ will be on an absolute scale, will be assigned a sigma of zero, a scale factor number of NSCALE + 1, and E1=E2=0.

Least Squares Output

Cards: FØRMAT(I1,F3.0,2F4.0,2F9.3,I3,7F6.3,F5.1)

ISENT,H1,H2,H3,FSQ,SIG,ISCALE,(E1(I) I=1,8)

Binary Tape: (TAPE 18 if written) ISENT,H1,H2,H3,FSQ,SIG,FSCALE,E1

The tapes will be properly terminated with ISENT = 1.

FSQ will be the original FSQ/SCALE(ISCALE) as determined from the Wilson plot. Ditto for SIG. All the other information is simply transcribed.

Fourier or Patterson output

No cards possible

Binary Tape (FØUR if written): IH,IK,IL,SINTHL,ORD,SHARP,COSWH,SINWH,SHNOO

Tapes are properly terminated with IH = 999

IH,IK,IL are transcribed indices.

SINTHL = sinθ/lambda

ORD = FSQ/SCALE(ISCALE)

SHARP = ORD * EXP(2.*B*SINTHL**2) * $\dfrac{\sum f_i^2(\sin\theta/\lambda = 0)}{\sum f_i^2(\sin\theta/\lambda)}$

SHNOO = SHARP - $\sum f_i^2[(\sin\theta/\lambda) = 0]$

CONTROL CARDS ON PATTERSON (JIMDAP) ARE THEN

Ordinary Patterson:	00022
Sharp Patterson:	00023
Origin Removed: and sharpened	00020

Note that unobserved reflections including space group extinctions should be included if an origin-removed Patterson is to be run.

Variable Subroutines

IMP

If IC(4) = 2, the user must supply an additional data card following card 6. This card must specify the FØRMAT in which the data is to be read. The parentheses are necessary, and 72 columns are available. If this card is blank, the default FØRMAT is identical to that of ECSØRTH output (I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3,F5.1).

```
      SUBROUTINE IMP(ISENT,H1,H2,H3,FSQ,SIG,SCALEN,E1,E2)
C     STANDARD IMP ROUTINE WILL READ FROM FILE DATA IN FORMAT
C     SPECIFIED ON OPTIONAL CARD 7 IN INPUT.
C     DEFAULT FORMAT IS THAT OUTPUT BY ECSORTH (TAPE3).
C     DEFAULT IS USED WHEN CARD 7 IS BLANK.
      DIMENSION E1(25)
      INTEGER DATFOR(12)
      DATA IFIRST/0/
      IF(IFIRST.NE.0) GO TO 2
      READ(5,1) DATFOR
    1 FORMAT(12A6)
    2 IF(DATFOR(1).EQ. 6H       ) GO TO 4
      READ (15,DATFOR) ISENT,H1,H2,H3,FSQ,SIG,SCALEN,(E1(I),I=1,8)
      IFIRST=1
      RETURN
    4 READ(15,3) ISENT,H1,H2,H3,FSQ,SIG,SCALEN,(E1(I),I=1,8)
    3 FORMAT(I1,F3.0,2F4.0,2F9.3,F3.0,7F6.3,F5.1)
      IFIRST=1
      RETURN
      END
```

WEIGHT - weight is called by XDATA for each reflection
Data is not weighted for the Wilson plot. Reflections may however be rejected.

```
SUBRØUTINE WEIGHT (H1,H2,H3,F,SIG,SCALEN,E1,E2,INØN)
DIMENSION E1(25)
SET INØN= 1  if reflection is not to be used in Wilson Plot.
SET INØN= 0  if reflection is to be used in Wilson Plot.
```

Deck Setup

ATTACH(XDATA,XDATA,ID=CPRØGS)

FTN(SYSEDIT) if any compilations

Tape requests if any.

LØAD(LGØ) if necessary

XDATA.

Rewind tapes etc.

7/8/9

Source decks for WEIGHT and IMP if required

7/8/9 if required for compilation termination

Data as described above

6/7/8/9

APPENDIX 3. PROTEIN DATA BANK FILE FORMAT

PROTEIN DATA BANK

FILE RECORD FORMATS

July 1976

MACROMOLECULAR STRUCTURE FILE

For each parameter set the file consists of records each of 80 characters.

The record sequence is as follows:-

HEADER	:	Date entered into data bank; identification code.
COMPND	:	Name of protein and identifying information
SOURCE	:	Species from which protein has been obtained
AUTHOR	:	Names of contributor and coauthors
JRNL	:	Literature citation which defines coordinate set
REMARK	:	General remarks
SEQRES	:	The residue sequence
FTNOTE	:	Footnotes relating to specific atoms or residues
HET	:	Identification of non-standard groups
HELIX	:	Identification of helical substructures
SHEET	:	Identification of sheet substructures
TURN	:	Identification of hairpin turns (β bends)
SITE	:	Identification of groups comprising the various sites
CRYST1	:	Unit cell data
ORIGX	:	Transformation matrix (orthogonal Å coords → submitted coords)
SCALE	:	Transformation matrix (orthogonal Å coords → fractional crystallographic coords)
MTRIX	:	Transformation matrix (expression of non-crystallographic symmetry)
ATOM	:	Atomic coordinate records
HETATM	:	Coordinates for heterogenous components
TER	:	Chain terminator
CONECT	:	Connectivity records
MASTER	:	Master control record with checksums of total number of records in the file, broken down by record type
END	:	End of data record

In describing record formats it will be convenient to use the punched-card analogy and refer to column numbers.

RECORD FORMATS

1. HEADER Cols. 1-6 HEADER
   11-50 Reserved for future use
   51-60 Date entered into data bank
   63-70 Identification code

   FORMAT (6A1,4X,60A1)

   Note: Each macromolecule is assigned an identification code. The code consists of 1 numeric and 3 alphabetic characters. The former is provided to distinguish multiple data sets for the same macromolecule.

2. COMPND Cols. 1-6 COMPND
   11-70 Name of molecule

   FORMAT (6A1,4X,60A1)

3. SOURCE Cols. 1-6 SOURCE
   11-70 Species from which molecule has been obtained

   FORMAT (6A1,4X,60A1)

4. AUTHOR Cols. 1-6 AUTHOR
   11-70 Names of contributor and coauthors

   FORMAT (6A1,4X,60A1)

5. JRNL Cols. 1-4 JRNL
   11-70 Literature citation which defines the coordinate set

   FORMAT (6A1,4X,60A1)

6. REMARK Cols. 1-6 REMARK
   8-10 Remark number
   12-70 Remarks

   FORMAT (6A1,1X,I3,60A1)

   Note: - The first REMARK has serial number 1, the second 2, etc.

7. SEQRES Cols. 1-6 SEQRES
   9-10 Serial number
   12 Chain identifier
   14-17 No. of residues in this chain
   20-22 Residue name
   24-26 Residue name
   ⋮
   68-70 Residue name

   FORMAT (6A1,I4,1X,A1,1X,I4,1X,13(1X,A3))

   Serial numbers are reset to 1 for each new chain.

8. FTNOTE

Cols.	1-6	FTNOTE
	8-10	Footnote number
	12-70	Footnote statement

FORMAT (6A1,1X,I3,60A1)

Note: - FTNOTE records are used to describe details which are specific to certain atoms or residues. These footnotes are keyed to particular atoms by the footnote number here and in cols 68-70 of the ATOM record. Any individual footnote may run over several FTNOTE records (each with the same footnote number).

9. HET

Cols.	1-3	HET
	8-10	Heterogen identifier
	12-18	Sequence identifier (see page 8)
	21-25	No of atoms in heterogenous group
	31-70	Text

FORMAT (6A1,1X,A3,2X,A1,I4,A1,2X,I5,5X,40A1)

10. HELIX

Cols.	1-6	HELIX	
	8-10	Serial number (Helix number)	
	12-14	Helix identifier (right justified)	
	16-18	Residue name	Initial residue of helix
	20	Chain identifier	Initial residue of helix
	22-25	Residue seq. no.	Initial residue of helix
	26	Insertion code	Initial residue of helix
	28-30	Residue name	Terminal residue of helix
	32	Chain identifier	Terminal residue of helix
	34-37	Residue seq. no.	Terminal residue of helix
	38	Insertion code	Terminal residue of helix
	39-40	Class of helix (Appendix A)	
	41-70	Remarks	

FORMAT (6A1,1X,I3,1X,A3,1X,A3,1X,A1,1X,I4,A1,1X,A3,1X,A1,1X,I4,A1,I2,30A1)

Notes: (i) The initial residue has a lower sequence number than the terminal residue.

(ii) Additional records with different serial numbers and identifiers occur if more than one helix is present.

11. <u>SHEET</u> Cols. 1-5 SHEET

8-10	Strand number[(i)(v)]	
12-14	Sheet identifier[(i)] (right justified)	
15-16	Number of strands	
18-20	Residue name	Initial residue
22	Chain identifier	
23-26	Residue seq. no.[(ii)]	
27	Insertion code	
29-31	Residue name	Terminal residue
33	Chain identifier	
34-37	Residue seq. no.	
38	Insertion code	
39-40	Sense of above strand with respect to previous strand[(iii)]	
42-45	Atom name	Registration[(iv)]
46-48	Residue name	
50	Chain identifier	
51-54	Residue seq. no.	
55	Insertion code	
57-60	Atom name	Registration[(iv)]
61-63	Residue name	
65	Chain identifier	
66-69	Residue seq. no.	
70	Insertion code	

FORMAT (6A1,I4,1X,A3,I2,2(1X,A3,1X,A1,I4,A1),I2,2(1X,A4,A3,1X,A1,I4,A1))

<u>Notes</u>:

(i) Different strands are described in subsequent records which bear the same sheet identifier but different strand numbers.

(ii) The initial residue of a strand has a lower sequence number than the terminal residue.

(iii) Parallelism or anti-parallelism of strand n with respect to strand n-1 is denoted by 1 or -1. Strand 1 has sense indicator 0.

(iv) Registration of the strand n with respect to strand n-1 may be specified by a particular hydrogen bond between the indicated atoms. One donor and one acceptor should be specified. These fields will be blank for strand 1.

(v) Strand numbers are reset to 1 for the first strand of each new sheet. A closed sheet (β barrel) is indicated by having the first and last strands identical.

12. TURN

Cols.	1-5	TURN	
	8-10	Sequence number (Turn number)	
	12-14	Turn identifier (3 characters)	
	16-18	Residue name	Residue i
	20	Chain identifier	
	21-24	Residue seq. no.	
	25	Insertion code	
	27-29	Residue name	Residue i + 3
	31	Chain identifier	
	32-35	Residue seq. no.	
	36	Insertion code	
	41-70	Comment	

FORMAT (6A1,1X,I3,1X,A3,1X,A3,1X,A1,I4,1X,A1,A3,1X,A1,I4,A1,4X,30A1)

Note: - These records identify the hairpin turns (β bends) in the structure which do not occur in helices.

13. SITE

Cols.	1-4	SITE	
	8-10	Sequence no.(i)	
	12-14	Site identifier(ii) (right justified)	
	16-17	No. of residues comprising site(iii)	
	19-21	Residue name	First residue comprising site
	23	Chain identifier	
	24-27	Residue seq. no.	
	28	Insertion code	
	30-32	Residue name	Second residue comprising site
	34	Chain identifier	
	35-38	Residue seq. no.	
	39	Insertion code	
	41-43	Residue name	Third residue comprising site
	45	Chain identifier	
	46-49	Residue seq. no.	
	50	Insertion code	
	52-54	Residue name	Fourth residue comprising site
	55	Chain identifier	
	57-60	Residue seq. no.	
	61	Insertion code	

FORMAT (6A1,1X,I3,1X,A3,1X,I2,4(1X,A3,1X,A1,I4,A1))

Notes:
(i) Sequence numbers are reset to 1 for each new site.
(ii) Site identifiers should be fully explained in the REMARKs.
(iii) If a site is comprised of more than four residues then these may be specified on additional records bearing the same site identifier.

14. <u>CRYST1</u> Cols. 1-6 CRYST1

7-15	a(Å)
16-24	b(Å)
25-33	c(Å)
34-40	α(deg.)
41-47	β(deg.)
48-54	γ(deg.)
56-66	Space group symbol (left justified)
67-70	Z

FORMAT (6A1,3F9.3,3F7.2,1X,11A1,I4)

15. <u>ORIGX</u> Cols.

1-6	11-20	21-30	31-40	46-55
ORIGX1	O_{11}	O_{12}	O_{13}	T_1
ORIGX2	O_{21}	O_{22}	O_{23}	T_2
ORIGX3	O_{31}	O_{32}	O_{33}	T_3

FORMAT (6A1,4X,3F10.5,5X,F10.5)

<u>Note</u>: - Let the original submitted coordinates be $X_oY_oZ_o$

Let the orthogonal Å coordinates contained in the file be X,Y,Z

Then
$$X_o = O_{11}X + O_{12}Y + O_{13}Z + T_1$$
$$Y_o = O_{21}X + O_{22}Y + O_{23}Z + T_2$$
$$Z_o = O_{31}X + O_{32}Y + O_{33}Z + T_3$$

Even if this is an identity transformation (unit matrix, null vector it is supplied. See below under SCALE for a definition of the default orthogonal Å system. Appendix B details the derivation of this coordinate transformation.

16. <u>SCALE</u> Cols.

1-6	11-20	21-30	31-40	46-55
SCALE1	S_{11}	S_{12}	S_{13}	U_1
SCALE2	S_{21}	S_{22}	S_{23}	U_2
SCALE3	S_{31}	S_{32}	S_{33}	U_3

FORMAT (6A1,4X,3F10.5,5X,F10.5)

<u>Note</u>: - Let the orthogonal Å coordinates be X Y Z

Let the fractional cell coordinates be x y z

Then
$$x = S_{11}X + S_{12}Y + S_{13}Z + U_1$$
$$y = S_{21}X + S_{22}Y + S_{23}Z + U_2$$
$$z = S_{31}X + S_{32}Y + S_{33}Z + U_3$$

The SCALE transformation provides a means of generating fractional coordinates from the orthogonal Å coordinates contained in the file.

Unless otherwise specified in the REMARKs the orthogonal Å coordinate system is related to the axial system of the space group supplied (CRYST1 record) by the definition below.

If $\vec{A},\vec{B},\vec{C}$ are unit vectors in the orthogonal Å system and $\vec{a},\vec{b},\vec{c}$ are unit vectors in the crystallographic system then: -

(i) the $\vec{A},\vec{B},\vec{C}$ and $\vec{a},\vec{b},\vec{c}$ systems have the same origin

(ii) $\vec{A}$ is parallel to $\vec{a}$

(iii) $\vec{B}$ is parallel to $\vec{C} \times \vec{A}$

(iv) $\vec{C}$ is parallel to $\vec{a} \times \vec{b}$, (i.e. $\vec{c}^*$)

Appendix B details the derivation of this coordinate transformation.

17. <u>MATRIX</u>

Cols.	1-6	8-10	11-20	21-30	31-40	46-55
	MTRIX1	Serial no.	M_{11}	M_{12}	M_{13}	V_1
	MTRIX2	Serial no.	M_{21}	M_{22}	M_{23}	V_2
	MTRIX3	Serial no.	M_{31}	M_{32}	M_{33}	V_3

FORMAT (6A1,1X,I3,3F10.5,5X,F10.5)

<u>Note</u>: - In a structure with non-crystallographic symmetry, MTRIX records are used to generate coordinates for the full contents of an asymmetric unit. In some cases the full asymmetric unit is explicitly given and in these cases the MTRIX records simply describe the nature of the local symmetry operations.

Let orthogonal Å coordinates of a subunit contained in the file be X, Y, Z and coordinates of a particular related subunit be X', Y', Z'.

$$X' = M_{11}X + M_{12}Y + M_{13}Z + V_1$$
$$Y' = M_{21}X + M_{22}Y + M_{23}Z + V_2$$
$$Z' = M_{31}X + M_{32}Y + M_{33}Z + V_3$$

The serial number is constant for each group of three MTRIX records. More than one group of MTRIX records may be present to describe different local symmetry operations.

Appendix B details the derivation of this coordinate transformation.

18. <u>ATOM</u> Atomic coordinate records

Cols.	1-4	ATOM
	7-11	Atom serial number(i)
	13-16	Atom name(ii)
	17	Alternate location indicator(iii)
	18-20	Residue name(iv)
	21-27	Sequence identifier(v)
	31-38	X } Orthogonal Å coordinates
	39-46	Y } Orthogonal Å coordinates
	47-54	Z } Orthogonal Å coordinates
	55-60	Occupancy
	61-66	Temperature factor
	68-70	Footnote number

FORMAT (6A1,I5,1X,A4,A1,A3,1X,A1,I4,A1,3X,3F8.3,2F6.2,1X,I3)

<u>Note</u>: - (i) Atoms occur in order of their serial numbers which always increase starting from the N-terminal residue. Within each amino acid residue the atoms are ordered as indicated in Appendix C. If the residue sequence is known certain serial numbers may be omitted to allow for future insertion of any missing atoms. If the sequence is not reliably known these serial numbers are simply ordinals.

(ii) Appendix C

(iii) Alternate locations for atoms may be denoted by A, B, C, etc. here.

(iv) Standard residue names are given in Appendix D, other components are defined in HET records.

(v) The sequence identifier would be a composite field made up as follows:

Cols.	21	Reserved for future expansion
	22	Chain identifier, e.g. A for hemoglobin α chain
	23-26	Residue sequence number
	27	Code for insertions of residues, e.g. 66A,66B,etc

19. <u>HETATOM</u> Cols. 1-6 HETATM

7-70 as for ATOM records

20. <u>TER</u> Cols. 1-3 TER

7-11 Serial number

18-20 Residue name

21-27 Sequence identifier

FORMAT (6A1,I5,6X,A3,1X,A1,I4,A1)

<u>Note</u>: - TER records occur among the ATOM records, and are placed after the terminal atom of each chain. The residue defined on these TER records is the carboxy-terminal residue of the chain in question.

21. <u>CONECT</u> Connectivity records

Cols.	1-6	CONECT
	7-11	Serial number
	12-16	Covalent bond connectivity (serial number of bonded atoms)
	17-21	
	22-26	
	27-31	
	32-36	Hydrogen bond connectivity (Donor)
	37-41	
	42-46	
	47-51	Hydrogen bond connectivity (Acceptor)
	52-56	
	57-61	

FORMAT (6A1,11I5)

<u>Note</u>: - Serial numbers are identical to those in cols 7-11 of the ATOM/HETATM records and connectivity entries correspond to these serial numbers. For metal atoms, which may form more than four covalent bonds, a second CONECT record with the same serial number may be used. Either all or none of the connectivity of an atom must be specified.

22. <u>MASTER</u>

Cols.	1-6	MASTER
	11-15	Number of REMARK records
	16-20	Number of FTNOTE records
	21-25	Number of HET records
	26-30	Number of HELIX records
	31-35	Number of SHEET records
	36-40	Number of TURN records
	41-45	Number of SITE records
	46-50	Number of MTRIX records (ORIGX+SCALE+MTRIX)
	51-55	Number of ATOM records (ATOM+HETATM)
	56-60	Number of TER records
	61-65	Number of CONECT records
	66-70	Number of SEQRES records

FORMAT (6A1,5X,12I5)

<u>Note</u>: - The MASTER record gives checksums of the number of records in the file, broken down by record type.

23. <u>END</u> End of data record

Cols. 1-3 END

FORMAT (6A1)

APPENDIX A

Classification of Helical Substructures

Class	Substructure
1	Right-handed α
2	Right-handed ω
3	Right-handed π
4	Right-handed γ
5	Right-handed 3_{10}
6	Left-handed α
7	Left-handed ω
8	Left-handed γ
9	2_7 Ribbon/helix

Default is class 1.

APPENDIX B

Coordinate Transformations

Usually the depositor will have supplied--

(i) The original submitted coordinates, i.e. $\vec{X}_o$

(ii) A transformation from $\vec{X}_o$ to the orthogonal Å coordinates stored in the data bank ($\vec{X}$)

i.e. $\underset{\sim}{O}_o \vec{X}_o + \vec{T}_o = \vec{X}$

where the subscripts denote "in the space of the original coordinates".

The default $\underset{\sim}{O}_o, \vec{T}_o$ transformation which transforms fractional crystallographic coordinate into the default orthogonal Å system is

$$\underset{\sim}{O}_o = \begin{pmatrix} a & b\cos\gamma & c\cos\beta \\ 0 & b\sin\gamma & c(\cos\alpha-\cos\beta\cos\gamma)/\sin\gamma \\ 0 & 0 & V/(ab\sin\gamma) \end{pmatrix}, \quad \vec{T}_o = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(iii) A transformation from $\vec{X}_o$ to fractional crystallographic coordinates ($\vec{x}$)

i.e. $\underset{\sim}{S}_o \vec{X}_o + \vec{U}_o = \vec{x}$

(iv) A set of transformations expressing any non-crystallographic symmetry elements in the structure

i.e. $\underset{\sim}{M}_o \vec{X}_o + \vec{V}_o = \vec{X}_o'$

Since it is desirable for the stored ORIGX, SCALE and MTRIX transformations to operate on the stored rather than the submitted coordinates some manipulation of the supplied quantities is performed in order to obtain the stored quantities.

The stored quantities are

(i) The coordinates in orthogonal Ångstroms ($\vec{X}$)

$$\vec{X} = \underset{\sim}{O}_o \vec{X}_o + \vec{T}_o$$

(ii) The ORIGX transformation from stored to original coordinates ($\underset{\sim}{O}$, $\vec{T}$).

From above $\vec{X} = \underset{\sim}{O}_o \vec{X}_o + \vec{T}_o$

whence $\underset{\sim}{O}_o \vec{X}_o = \vec{X} - \vec{T}_o$

$$\therefore \quad \vec{X}_o = \underset{\sim}{O}_o^{-1}\vec{X} + (-\underset{\sim}{O}_o^{-1}\vec{T}_o)$$

Thus $\underset{\sim}{O} = \underset{\sim}{O}_o^{-1}$

and $\vec{T} = -\underset{\sim}{O}_o^{-1}\vec{T}_o$

(iii) The SCALE transformation from stored to fractional coordinates ($\underset{\sim}{S}$, $\vec{U}$).

From above $\vec{x} = \underset{\sim}{S}_o \vec{X}_o + \vec{U}_o$

but $\vec{X}_o = \underset{\sim}{O}_o^{-1}\vec{X} + (-\underset{\sim}{O}_o^{-1}\vec{T}_o)$

$$\therefore \quad \vec{x} = \underset{\sim}{S}_o[\underset{\sim}{O}_o^{-1}\vec{X} + (-\underset{\sim}{O}_o^{-1}\vec{T}_o] + \vec{U}_o$$

i.e. $\vec{x} = \underset{\sim}{S}_o\underset{\sim}{O}_o^{-1}\vec{X} + (-\underset{\sim}{S}_o\underset{\sim}{O}_o^{-1}\vec{T}_o) + \vec{U}_o$

$$\therefore \quad \underset{\sim}{S} = \underset{\sim}{S}_o\underset{\sim}{O}_o^{-1}$$

and $\vec{U} = -(\underset{\sim}{S}_o\underset{\sim}{O}_o^{-1}\vec{T}_o) + \vec{U}_o$

(iv) The MTRIX transformation(s) expressing non-crystallographic symmetry in the space of the stored coordinates (M, $\vec{V}$).

$$\vec{X}_o' = \underset{\sim}{M}_o\vec{X}_o + \vec{V}_o$$

$$\therefore \quad \vec{X}' = \underset{\sim}{O}_o\vec{X}_o' + \vec{T}_o$$

$$= \underset{\sim}{O}_o\left\{\underset{\sim}{M}_o\vec{X}_o + V_o\right\} + \vec{T}_o$$

but $\vec{X}_o = \underset{\sim}{O}_o^{-1}\vec{X} + (-\underset{\sim}{O}_o^{-1}T_o)$

$$\therefore \quad \vec{X}' = \underset{\sim}{O}_o\left\{\underset{\sim}{M}_o[\underset{\sim}{O}_o^{-1}\vec{X} + (-\underset{\sim}{O}_o^{-1}T_o)] + \vec{V}_o\right\} + \vec{T}_o$$

$$\therefore \quad \underset{\sim}{M} = \underset{\sim}{O}_o\underset{\sim}{M}_o\underset{\sim}{O}_o^{-1}$$

and $\vec{V} = -\underset{\sim}{O}_o\underset{\sim}{M}_o\underset{\sim}{O}_o^{-1}\vec{T}_o + \underset{\sim}{O}_o\vec{V}_o + \vec{T}_o$

In summary the stored coordinates and transformations are:

$\vec{X}$	(ATOM records)
$\underset{\sim}{O},\vec{T}$	(ORIGX ")
$\underset{\sim}{S},\vec{U}$	(SCALE ")
$\underset{\sim}{M},\vec{V}$	(MTRIX ")

APPENDIX C

Atom Identifiers

Atom names, remoteness codes and order indicators for the common amino acids.

These atom names follow the IUPAC-IUB rules[1] except:

(i) Greek letter remoteness codes are transliterated according to the following table

α-A	δ-D	η-H
β-B	ε-E	
γ-G	ζ-Z	

(ii) Atoms for which some ambiquity exists in the crystallographic results are designated A. This will usually apply only to the terminal atoms of asparagine and glutamine and to the ring atoms of histidine.

Within each residue the atoms occur in the order specified by the superscripts (following figure).

The "extra" oxygen atom of the carboxy terminal amino acid is designated OXT.

Four characters are reserved for these atom names--they are assigned as follows:

1-2	Chemical symbol - right justified
3	Remoteness indicator (alphabetic)
4	Branch designator (numeric)

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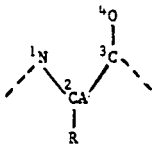
[1] IUPAC-IUB Commission on Biochemical Nomenclature. "Abbreviations and Symbols for the Description of the Conformation of Polypeptide Chains. Tentative Rules (1969)," Biochemistry, 9, 3471 (1970).
The 1974 recommendations on the "Nomenclature of α-Amino Acids" (Biochemistry, 14, 449 (1975)) provides a scheme based on normal rules for organic compounds but this scheme will not be used here.

Atom Names, Remoteness Codes, and Order Indicators for the Common Amino Acids

backbone



Name	Side Chain
Alanine	—5CB
Arginine	—5CB—6CG—7CD—8NE—9CZ (10NH1, 11NH2)
Asparagine	—5CB—6CG (7AD1 (OD1), 8AD2 (ND2))
Aspartic acid	—5CB—6CG (7OD1, 8OD2)
Cysteine/Cystine	—5CB—6SG
Glutamic Acid	—5CB—6CG—7CD (8OE1, 9OE2)
Glutamine	—5CB—6CG—7CD (8AE1 (OE1), 9AE2 (NE2))
Glycine	—null
Histidine	—5CB—6CG (7AD1 (ND1)—9AE1 (CE1), 8AD2 (CD2)—10AE2 (NE2))
Hydroxyproline	—(1N)—(2CA)— (7CD, 5CB, 6CG, 8OD)
Isoleucine	—5CB (7CG2, 6CG1—8CD1)

Name	Side Chain
Leucine	—5CB—6CG (3CD2, 7CD1)
Lysine	—5CB—6CG—7CD—8CE—9NZ
Methionine	—5CB—6CG—7SD—8CE
Phenylalanine	—5CB—6CG (7CD1—8CE1, 11CZ, 9CD2—10CE2)
Proline	—(1N)—(2CA)— (7CD, 5CB, 6CG)
Serine	—5CB—6OG
Threonine	—5CB (7OG1, 6CG2)
Tryptophan	—5CB—6CG (7CD1, 9NE1, 8CD2—10CE2, 11CE3, 12CZ2, 13CZ3—14CH2)
Tyrosine	—5CB—6CG (7CD1—8CE1, 11CZ—12OH, 9CD2—10CE2)
Valine	—5CB (6CG1, 7CG2)

APPENDIX D

Residue Names and Abbreviations

Residue	Abb.	Syn.	Residue	Abb.	Syn.
Acidic unknown	ACD		Homoserine	HSE	
Acetyl	ACE		Hydroxyproline	HYP	
Alanine	ALA		Hydroxylysine	HYL	
β-Alanine	ALB		Isoleucine	ILE	
Aliphatic unknown	ALI		Leucine	LEU	
γ-Aminobutyric acid	ABU		Lysine	LYS	
Arginine	ARG		Methionine	MET	
Aromatic unknown	ARO		Ornithine	ORN	
Asparagine	ASN		Phenylalanine	PHE	
Aspartic acid	ASP		Proline	PRO	
ASP/ASN ambiguous	ASX		Pyrollidone carboxylic acid	PCA	
Basic unknown	BAS		Sarcosine	SAR	
Betaine	BET		Serine	SER	
Cysteine	CYS	CYH,CSH	Taurine	TAU	
Cystine	CYS	CSS	Terminator	TER	
Formyl	FOR		Threonine	THR	
Glutamic acid	GLU		Thyroxine	THY	
Glutamine	GLN		Tryptophan	TRP	TRY
GLU/GLN ambiguous	GLX		Tyrosine	TYR	
Glycine	GLY		Unknown	UNK	
Heterogen	HET		Valine	VAL	
Histidine	HIS		Water	HOH	H2O,WAT

Note: - Standard residue abbreviations conform to the IUPAC-IUB rules in J. Biol. Chem., 241, 527, 2491 (1966).
Recognizable synonyms, such as those above, will be changed to the standard abbreviation.