

A COMPUTER-CONTROLLED NEUTRON TIME-OF-FLIGHT SPECTROMETER

S. H. Merriman

MASTER



OAK RIDGE NATIONAL LABORATORY

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MATHEMATICS DIVISION

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NEUTRON TIME-OF-FLIGHT SPECTROMETER

S. H. Merriman

JULY 1973

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
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ABSTRACT

A time-of-flight spectrometer for neutron inelastic scattering research has been interfaced to a PDP-15/30 computer, using a library of programs developed for collecting and analyzing a variety of experimental data. This report includes brief descriptions of the spectrometer and interface hardware and provides a discussion of the programming involved.

INTRODUCTION

A versatile time-of-flight spectrometer, which utilizes a magnetically pulsed neutron beam, has been developed for inelastic neutron scattering investigations of liquids and solids. The beam is pulsed by changing the direction of the atomic magnetic moments in a ferrite crystal with an applied magnetic field. The single crystal serves as both the monochromator and pulser, and any type of pulse shape or length can be readily obtained because the pulsing is accomplished electronically. The pulse repetition rate can also be varied continuously so that the magnetic pulser can operate in any type of auto-correlation mode.

This magnetically pulsed time-of-flight spectrometer, developed by the Solid State Division, has been installed at the High Flux Isotope Reactor at The Oak Ridge National Laboratory.¹ It has been linked to a Digital Equipment Corporation PDP-15/30 computer by an interface which was designed and built by the Instrumentation and Controls Division.² The computer is used for on-line control of the experimental apparatus and data acquisition devices. A series of programs has been written to position accurately the monochromator, sample, and detectors by means

of pulsed motors; to perform data collections in a scan mode;³ to operate the magnetic pulser in the optimum manner for an experiment of chosen duration; to pulse the crystal according to a desired sequence; to collect and cross-correlate time-of-flight data; and to display, plot, and analyze these data.

In Section 2 of this report, the computer programming effort associated with this project is described in some detail with emphasis on instructing the reader in the use of the programs.* To provide background, this discussion is preceded by an abbreviated summary of the experimental apparatus.

*The programs for driving all positioning equipment and for collecting data in the scan mode were written by L. W. Gilley of the Mathematics Division. A very brief description of these programs is presented in Section 2 of this report. However, for a thorough discussion of the motor drive and scan programs and the motor drive hardware, the reader should consult reference 3 of this report.

SECTION 1

INSTALLATION HARDWARE

1.1 Spectrometer

Since the time-of-flight spectrometer makes use of the one remaining beam tube at the High Flux Isotope Reactor, it was designed with maximum flexibility. The necessity of a versatile neutron-scattering facility has resulted in an elaborate spectrometer with continuously variable incident wave-length and more efficient counting apparatus than other systems in use.

1.1.1 Magnetic Pulser

The primary feature distinguishing this spectrometer from others at the HFIR is the incorporation of the magnetic pulsing device⁴ which was mentioned earlier. The method of magnetically pulsing a neutron beam obviates high-speed rotating equipment. This method utilizes the magnetic intensity in a Bragg reflection, which depends on the orientation of the atomic magnetic moments relative to the scattering vector and becomes zero when the moments are directed along the scattering vector. The direction of magnetization in ferrite crystals can be switched rapidly with an external magnetic field so that these crystals can serve both as a neutron monochromator and pulser. Furthermore, the neutron pulse width and repetition rate can easily be varied by changing the current pulse that produces the external field. For most applications, such a continuously modulated beam makes the magnetic chopper much more efficient than a conventional rotating chopper. A complete discussion of the physical principles involved in the pulsed neutron beam can be found elsewhere in the article entitled "A Magnetically Pulsed Time-of-Flight Spectrometer for Inelastic Neutron Scattering."¹

1.1.2 Counting Equipment

Another difference between this spectrometer and other commonly used is the higher counting rate made possible by the inclusion of multiple detectors. Sixteen banks of high pressure ^3He neutron detectors can be used to provide as many separate data channels.

1.1.3 Spectrometer Hardware

A schematic drawing of the spectrometer appears in Fig. 1. The monochromator-pulser ferrite crystal is mounted at the center of a massive radiation shield which weighs 84,000 pounds and has a diameter of 92 inches. The sample and the flight-path assembly are attached to the monochromator shield so that the crystal scattering angle can vary between zero and ninety degrees. The flight-path assembly, weighing 3,650 pounds, is carried over the floor on three air bearings. The sixteen detectors are mounted on a track within the assembly and allow scattering angles from the sample of 10 to 140 degrees.

1.1.4 Positioning Equipment

All positioning of the apparatus is accomplished by means of pulsed motors which are controlled by the computer. There are at present five Slo-Syn stepping motors² which rotate the following components to the desired angular settings: the pulsing crystal, the sample, and each of the three detector mounts. A motor makes 200 steps per motor shaft revolution, resulting in a one degree movement of the accompanying spectrometer component about its axis. Thus, one motor step is equal to $1/200$ of one degree of spectrometer axis motion, which is equivalent to a positioning accuracy of $.005^\circ$. Each motor

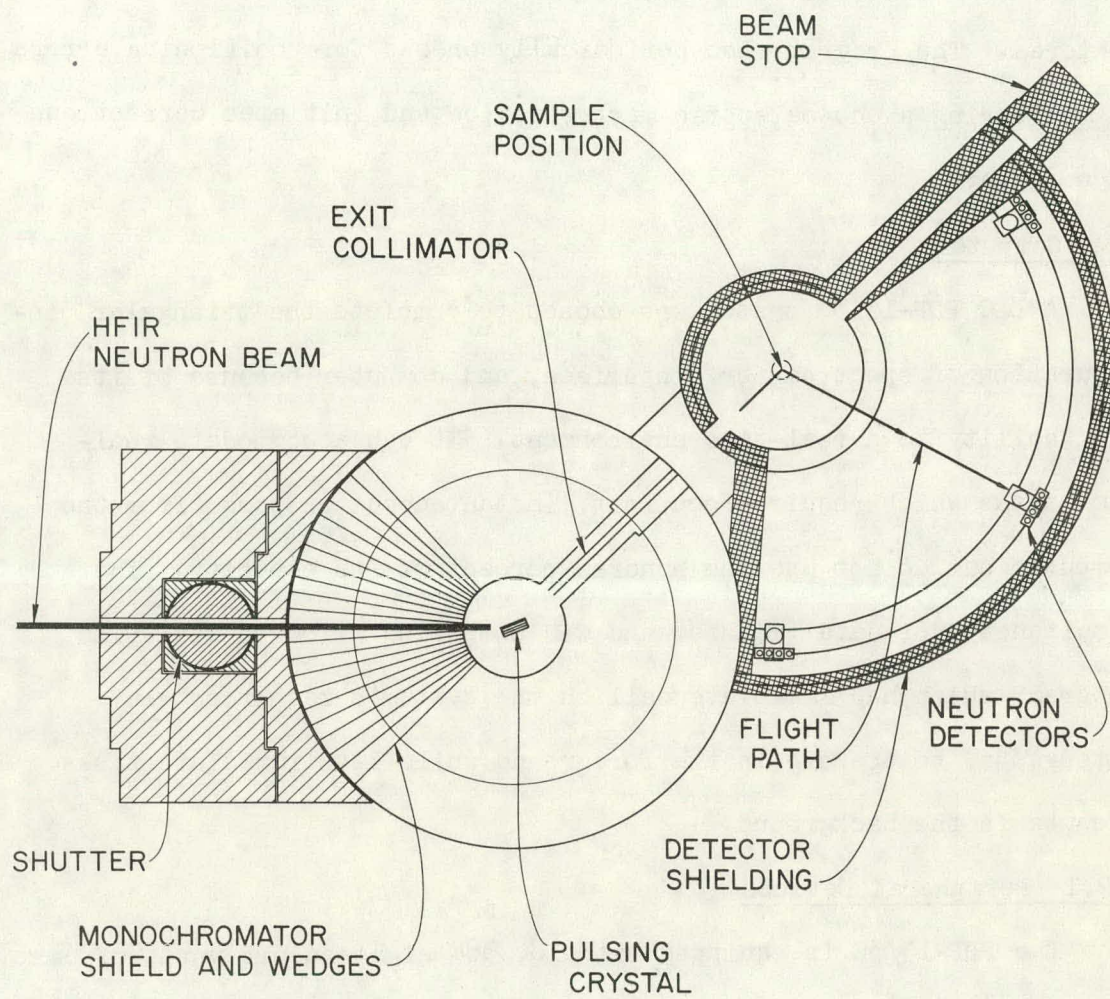


Fig. 1. Spectrometer

has two unique Input/Output Transfer (IOT) instructions for stepping the motor $.005^{\circ}$ backward or forward. A computer program (see Section 2.2), given the actual and desired motor shaft positions, drives the motor in the appropriate direction until the desired angular setting has been achieved. The program also periodically checks for positioning errors by monitoring a photoelectric marker device and initiates corrections if necessary.

1.2 Computer

A DEC PDP-15/30 system was chosen to complete the triangular configuration of spectrometer, interface, and computer because of its adaptability to a real-time environment. It can accommodate real-time tasks which require recurrent, instantaneous response from the computer but do not use one hundred percent of its capacity. The simultaneity of data transfer and CPU computing allows a real-time program, which has immediate call on the system's resources via interrupts, to operate in the foreground while less immediate tasks execute in the background.

1.2.1 Peripheral Devices

The PDP-15/30 is equipped with 16, 384 eighteen-bit words of core memory having an 800 nanosecond cycle time. The peripheral devices include two Teletypes, three DECTape transports, a DECdisk, a high speed paper tape reader and punch, a Hewlett-Packard oscilloscope display unit, and a Complot incremental plotter. The configuration also contains a real-time clock and an elaborate interrupt system. Since these last two components are necessary parts of any real-time system, perhaps a brief explanation of their hardware is appropriate.

1.2.2 Real-Time Clock

When enabled, the clock counts, in a dedicated memory location, the number of cycles completed by the line voltage (60 Hz) until the location overflows. At this time an interrupt request is generated, informing the monitor that the preset interval is over. The monitor must either disable the clock or reinitialize the location to the 2's complement of the number of counts it needs to tally.

1.2.3 Interrupt Facilities

The priority of servicing interrupts is of great importance in a real-time system since frequently there are simultaneous requests for transferring information and the validity of the experiments depends on the order in which the interrupts are serviced. The Input/Output (I/O) processor always has priority over the CPU in accessing memory and the use of the common I/O bus is determined by the following order: block data transfers, real-time clock, Automatic Priority Interrupt, and Program Interrupt.

Block Data Transfers

Normally, three data channels are used for multi-cycle block transfers. The three devices to which these channels are assigned will be discussed in detail in the Interface section (Section 1.3). Each channel has two words reserved in core for storing the number of words to be moved and the current address. The data transfer is initiated by an IOT instruction after the two core locations have been set. The I/O Processor continues to transfer information until the word count register overflows causing an interrupt at a preassigned

API level. Because these multi-cycle block transfers are completely automatic in nature and do not require any CPU attention except the IOT initialization, the CPU is free for computation while they are taking place.

Automatic Priority Interrupt (API)

The API facility provides for servicing all devices except the primary Teletype and the Complot plotter, which are tied to the Program Interrupt. The Automatic Priority Interrupt system has eight priority levels, the lower four (4-7) being allocated to software and the higher four (0-3) to hardware. Each level, in turn, can have up to eight independent interrupts. Four of these are committed to servicing programmed requests leaving the remainder for I/O devices. The four software levels are used to establish a priority queue for data processing without inhibiting the hardware interrupts.

The API hardware guarantees that simultaneous requests by multiple devices are handled in the proper order. Higher priority interrupt requests are handled first, while holding lower priority requests off-line until they can be serviced. A typical sequence is as follows: an I/O device requests service by transmitting an interrupt request signal to the processor on a line corresponding to its unique, pre-assigned priority level. If this level is higher than that of the device which requested the currently active program, an interrupt is granted the new device. Upon receipt of the grant signal, the device transmits its channel address back to the CPU. The address serves as the entry point (trap address) to the device's service routine. After

debreaking from the service program, the API hardware returns control to the previously executing program unless, meanwhile, a higher device has raised its flag. If two or more requests are made concurrently on the same level, the device controller nearest the processor is given priority.

Proper use of the API software levels allows necessary calculations to be made without disturbing the flow of data. The software levels, in the case of this particular installation, are used for system monitor communication (such as user commands and error messages), sorting of incoming time-of-flight data, and displaying the data. Since these functions are secondary to the collection of data and re-initialization of interface and other devices, the programs performing these functions are normally allowed to remain at their preset software levels. However, under program control, a priority request can be raised to a higher level than the one to which it was assigned in order to complete necessary computations without interruption from I/O devices.

Program Interrupt

The Program Interrupt facility relieves the user program of the need for repeated checks of I/O device flags by allowing the ready status of device flags to cause automatically a program interrupt. The CPU continues execution of a program until a device flag is raised. At that time, the program is interrupted and control is transferred to an I/O service routine for IOT instructions. All vital information for returning CPU operation to pre-interrupt status is automatically

stored in location 0. The service routine must determine which peripheral device requested service, perform the appropriate service function, and restore control to the interrupted program segment.

A complete description of the priority systems for the PDP-15 is found in The PDP-15 Systems Reference Manual.⁵

1.3 Interface

In addition to the standard devices which are interfaced to the PDP-15/30, there are several special devices designed and built by the Instrumentation and Controls Division. Only the devices designed specifically for this installation will be discussed here. This discussion will be limited to the programming aspects and the reader should see "Control System Description Neutron Time-of-Flight Spectrometer"² for more extensive information on the hardware design. All other devices are described completely in the PDP-15 systems literature.

Figure 2 is a simplified schematic of the interface structure showing the interaction of the five primary devices: the Programmed Pulse Generator, Time-of-Flight Scaler, Interrupt Register, Prescaler, and Motor Drive Assembly.

1.3.1 Programmed Pulse Generator (PPG)

The PPG is responsible for pulsing the neutron beam according to a specified pseudorandom binary code. The code, fitting the specifications of the experiment, is chosen from a series of files stored on DEctape and read into a buffer in memory. While the experiment is in progress, the PPG gets the coded sequence (one word at a time via multicycle data channel) from memory and operates the pulsing crystal according to that sequence.

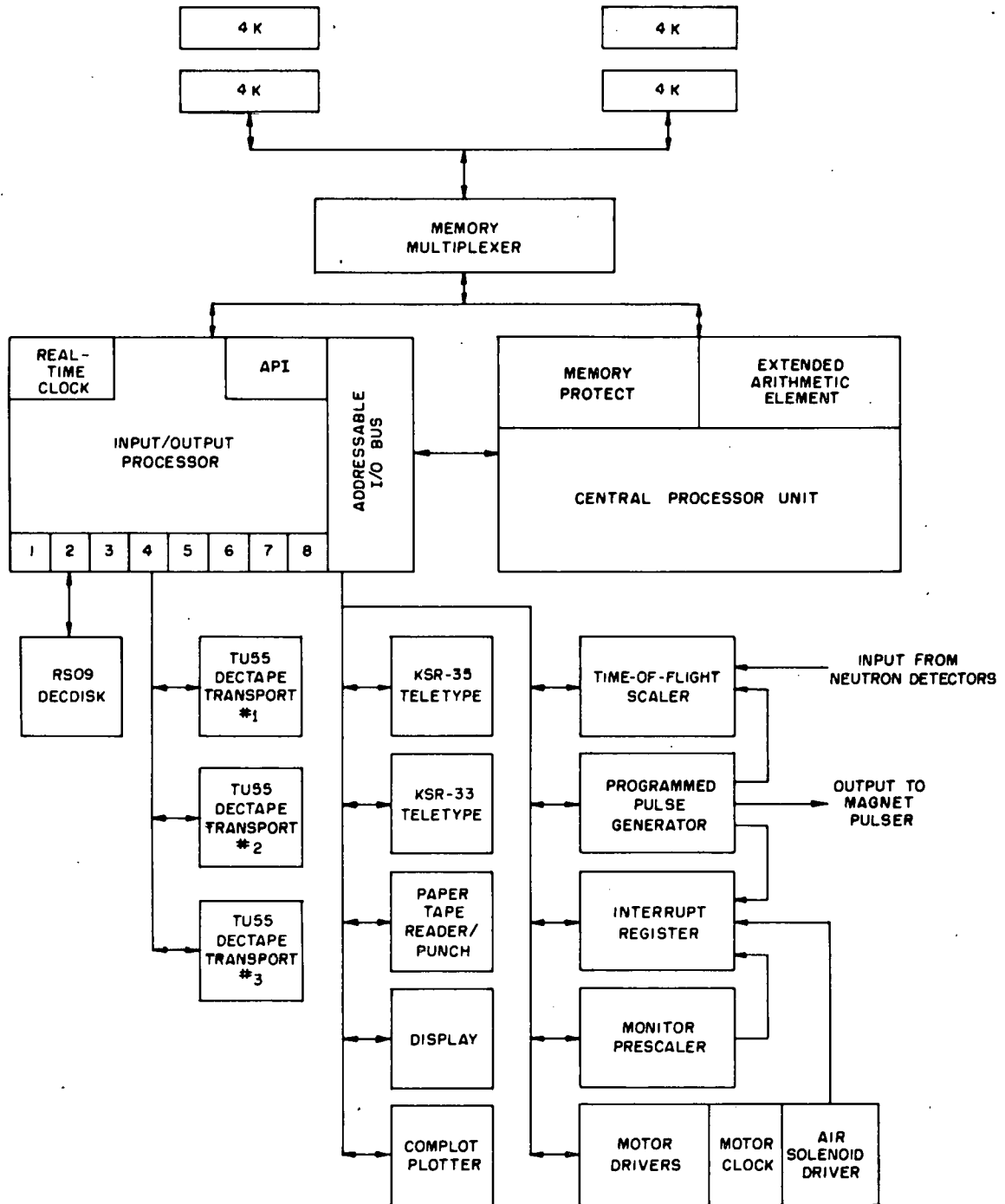


Fig. 2. Schematic of the Interface Structure

To ensure proper data collection, the PPG must be serviced immediately when an interrupt request occurs. Therefore, it has been assigned to API level 0 and has a priority status second only to that of the Power Fail facility. As a part of the initialization procedure before an experiment begins, the computer program places the word count (WC) and the current address (CA) of the coded sequence into locations 26_8 and 27_8 respectively. (See Table 1 in Appendix A.) It also stores a JMS (Jump to Subroutine instruction) to the PPG service routine in location 65_8 , which is the preset trap address. Coded data is transmitted between memory and pulsing apparatus through the data channel (without hindering the CPU) until the WC register overflows, raising the PPG interrupt flag. This causes an automatic "trap" to location 65_8 and therefore a jump to the service program. The PPG service routine immediately reinitializes the WC and CA, clears the overflow flag, and debreaks to the next highest priority where a device has requested service.

The PPG assembly includes three hardware registers called the Status Register, A Register, and B Register.

Status Register

A status word is transferred by IOT instruction to the Status Register in the PPG before an experiment is begun and resides in the PPG for the duration of the experiment. The status word consists of several input parameters which are packed as follows: bits 6-17 contain the 2's complement of the number of elements in the binary sequence. Bit 5, when set to "1", signals that the PPG is not enabled and that

the Time-of-Flight Scaler will operate in the scan mode. In many cases this scan will be along a symmetry axis of the sample crystal. In this mode no time information is transferred to the computer with the detector events - only the detector identification. (See Section 2.2.) When bit 4 is set, the PPG is informed that the number of bits in the sequence is less than or equal to 36. Setting this bit ensures that only one PPG data channel cycle need be executed during the experiment because the entire sequence is stored in the PPG hardware registers (A and B). This action allows for more efficient data collection since the PPG is not constantly requesting service on API level 0 and, hence, shutting out the TOF Scaler which interrupts at a lower priority. Bit 3 is set equal to the last sequence bit for error detection purposes during an experimental run. Bits 1 and 2 establish the number of time-of-flight channels per element of pseudorandom code.

<u>Bit 1</u>	<u>Bit 2</u>	<u>Channels/Element</u>
0	0	1
0	1	2
1	0	4

Bit 0, when initialized to "1", places the PPG in a single step diagnostic mode. The PPG can be stepped through the sequence one element at a time by a special IOT instruction. The contents of the hardware registers can be transferred to the Accumulator so that a comparison can be made with corresponding bits in memory. Artificial detector pulses are generated, giving an apparent event per channel for each

Scaler. In this way, PPG and TOF Scaler data are transferred via data channel as in normal operation, but at a rate commensurate with the rate of execution of the diagnostic IOT.

A Register

The A Register holds the first eighteen elements of the sequence and is set as a part of the pre-experiment initialization process. This word need never be addressed by the data channel since it resides in the PPG and, therefore, the PPG current address is always initialized to the second word in the sequence. The reason for having the A Register is to allow the PPG and TOF service routines sufficient time to execute even if there happens to be only one bit of sequence information in the last word. Bit 17 of the A Register contains the first bit of the sequence and bit 0 contains the eighteenth bit of the sequence.

B Register

The remaining elements of the sequence (eighteen bits at a time upon request from the data channel) pass through the B register in a continuous cycle until the experiment is terminated.

1.3.2 Time-of-Flight (TOF) Scaler

The TOF Scaler module collects the uncorrelated time-of-flight data and identifies them for subsequent sorting. The TOF unit is controlled by and synchronized with the PPG by three coaxial cables on the front panel of the interface cabinet. These are a "RUN" enable signal which activates the Scaler when the PPG is enabled; a "SYNC" signal which resets the Scaler to zero at the beginning of each sequence; and a "CLOCK" signal which advances the Scaler.²

There are sixteen 12-bit registers and flags, one of each being dedicated to a neutron detector. When a pulse arrives from a detector,

the time (within the sequence) is stored in the corresponding register. A scanner examines the flags sequentially at the rate of one every forty microseconds. When it locates a detector having a raised flag, a data channel transfer of the time channel (twelve bits) and detector identification (four bits) is requested. This information is gated through the output multiplexer to the computer where the data sorting program expects to find one word of information for each event. Bits 14-17 contain the detector identification, bits 2-13 the time channel, and bits 0 and 1 are unused at this time. The maximum allowable number of time channels (and, hence elements in the sequence) is 4096. A switch on the interface panel allows the user to select all sixteen detectors or a smaller grouping (2, 4, or 8). Since the maximum total count rate is a constant (25,000 counts per second), higher rates per detector can be attained by choosing a smaller group.

These data are temporarily stored in one of two 400_g word buffers in core. While one region is being filled, a low priority (API level 4) segment is sorting and storing the other.

The TOF Scaler has the third highest priority in the system, following the Power Fail Option and PPG. Its API level is 0 and the WC and CA registers are 34_g and 35_g. When one of the two data buffers is filled, location 34_g overflows causing an automatic entry to the TOF service routine (trap address is 76_g). This program switches data buffers so that the full buffer can be sorted while the second buffer receives data. After clearing the TOF flag, a debreak to software level 4 is executed, initiating the sort program. The sorting, of

course, does not inhibit PPG and TOF functions since they are being performed at a higher level. The sorting program must be efficient enough to handle one detector at the maximum rate of 25,000 counts per second, so that the time required for sorting 400 words of data is not greater than that required to collect 400 words. The time left after sorting one buffer and before sorting the other is used for displaying the raw TOF data. This monitoring of the data allows operator awareness of the progress of the experiment and on-line corrections where needed.

1.3.3 Interrupt Register (IR)

The IR module provides an interrupt capability for up to sixteen devices. It is assigned to API level 2 and its service routine trap address is location 77g. Each of the sixteen bits of the IR is identified with a given device by attaching BNC cables² to the appropriate input connector of the front panel of the interface cabinet. When one or more bits are set in the IR, an interrupt request is initiated on level 2. The service program, after transferring the contents of the IR to the Accumulator, executes a shift and test procedure for identifying the individual interrupt flag. (See Table 3 in Appendix A for corresponding device and Accumulator position.)

Only three of these flags have any significance in the normal data collection mode. The others, including six motor degree marker signals and motor clock interrupt signal, are of importance only in the motor drive and scan mode operations and will not be discussed here.³

Two of the three flags to be considered in normal data collection are PPG error signals. A "Sequence" error occurs when the final bit

in the sequence does not agree with bit 3 of the PPG Status Register. The Sequence error causes bit 16 in the IR to be set. No action is taken until ten successive errors have occurred. A "Lag" error (causing bit 15 in the IR to be set) indicates that data has not been loaded into the B register at a fast enough rate. Bit 1 is used to specify interrupt requests from the incident beam Prescaler which will be discussed in the following section. After the IR service routine has determined which bit(s) was set and has taken appropriate steps, the IR flag is cleared and the experiment continues.

1.3.4 Monitor Prescaler

The Monitor Prescaler is part of a system which determines the length of an experiment as a function of the intensity of the incident neutron beam. If the Prescaler is enabled, the incident beam is monitored by a detector and a scaling factor of 64 to 8192 is selected. Pulses from the Prescaler cause API interrupts (via the IR) at a rate proportional to the beam intensity. After a preset number of Prescaler interrupts have occurred, the counting period is terminated.

1.3.5 Motor Drive Assembly

The Motor Drive module provides the capability of driving eight motors for equipment positioning. Computer control of the motors is accomplished through special IOT instructions and the IR. Each time a motor executes one shaft revolution, a degree photomarker signal is cabled to the IR, where a given bit is set. (See Table 3, Appendix A.) By monitoring interrupt requests generated in this way, the computer keeps track of all movements of the motors.

Timing for stepping the motors is provided by a 300 Hz motor clock. This clock interrupts the computer 300 times per second by posting a flag in the IR, thus supplying a uniform time base for motor activity.

SECTION 2

COMPUTER SOFTWARE

Programs for controlling the spectrometer are written predominately in MACRO-15 (the PDP-15 assembly language) with a few FORTRAN IV subroutines. The standard object code produced by the MACRO-15 assembler and the FORTRAN IV compiler is in a relocatable format acceptable to the PDP-15/30 Linking Loader. The separately assembled subroutines, which may have common parameters called global symbols, are linked with system and user library programs into an executable object task.

The operating system currently in use is the ADVANCED Monitor Software System V5A.⁶ Operating in conjunction with the Input/Output Programming System (IOPS), the Monitor provides an interface between user programs and peripheral hardware. The IOPS supplies device handlers and error routines for all standard peripherals. Through teleprinter commands, the Monitor allows programs to be created, stored, loaded, and executed, as well as dynamic modification of I/O device assignments.

The programming effort has produced to date seven programs which are in continuous use. Each of these, excluding the motor drive program which has been documented elsewhere and therefore will receive only cursory attention in this report, will be discussed in the following sections. Examples of output from the programs are reproduced in Appendix B.

2.1 Angle Calculation

The angle calculation program, ANGL, determines the positions to which each of the five stepping motors will be set. The angular settings from ANGL are input to the motor drive program which positions

the monochromator, sample, and three detector mounts accordingly.

Table 4 in Appendix A shows which motor is used for situating each component.

2.1.1 Keyboard Monitor Commands

After loading a program, the user communicates with the system through a Keyboard Service Routine which is entered by typing a CONTROL S. (A CONTROL S is printed on the Teletype as follows: `↑S.`) Each of the seven user programs has its own Keyboard Monitor Routine which consists of a Monitor Command Decoder and a repertoire of Keyboard Commands. After typing the CONTROL S, the user types a two-character command followed by a carriage return. A jump to the appropriate subroutine (whose name is identical to the two-character Keyboard Command) is executed, initiating the required function.

The Advanced Monitor Software System reserves a register (106_8) for the starting address of the user's program. In this instance, of course, the starting address of ANGL will be deposited in location 106 by the Linking Loader. A CONTROL S causes a jump to the address in 106 and, hence, the execution of ANGL. As a part of its initialization, ANGL places the starting address of the Keyboard Monitor Routine in 106 so that any subsequent typing of the CONTROL S causes an entry into the service routine which waits for a Keyboard Command. After the Keyboard Command is acted upon, control is returned to a waiting loop in ANGL until further commands are typed. A list of the Keyboard Commands available in ANGL is given in Table I.

2.1.2 Loading ANGL

The linking Loader is brought into core by the System Loader in response to a user request to the Resident Monitor. It is ready to accept a user command string after outputting a ">" to the teleprinter.

TABLE I

ANGL KEYBOARD COMMANDS

Command	Function
CB	Read Lattice Parameters
DS	Read Monochromator Spacing
XO	Choose Psi or Omega
M1	Mode 1 Input
M2	Mode 2 Input
M3	Mode 3 Input
M4	Mode 4 Input
CA	Calculate Angles
PA	Print Angles
RZ	Read Angle Corrections
PZ	Print Angle Corrections
Space Space	Stop and Reinitialize

All Keyboard Commands must be preceded by a CONTROL S and followed by a carriage return.

The loader input device is expected to be assigned to Device Assignment Table Slot minus 4 (DAT slot -4). After loading unconditionally all the programs which appear in the command string, the loader loads and links all requested and unresolved library programs. It first scans the user library (DAT slot -5) and then the system library (DAT slot -1).

The loading sequence for ANGL is as follows:*

```

LOADER
> ← ANGL (ALT MODE)
↑ S

```

The CONTROL S output by the loader signals a successful load and execution can begin when the user responds with a second CONTROL S.

2.1.3 ANGL Description

Figure 3 is a schematic of the system showing the angles computed by ANGL. The beam diffracted from the monochromator has a wavelength, λ_0 , determined by $2\theta_M$ and the spacing, d_M , of the diffracting planes. These neutrons have a momentum which is proportional to \vec{k}_0 ($|\vec{k}_0| = 2\pi/\lambda_0$) and an energy $E_0 \simeq |\vec{k}_0|^2$. The direction of \vec{k}_0 relative to some reference direction in the sample is specified by the angle ψ . Some of the neutrons are scattered through an angle ϕ_1 with a corresponding change in momentum, energy, and wavelength (\vec{k}', E', λ'). These neutrons are diffracted into a detector.

*The user response is underlined.

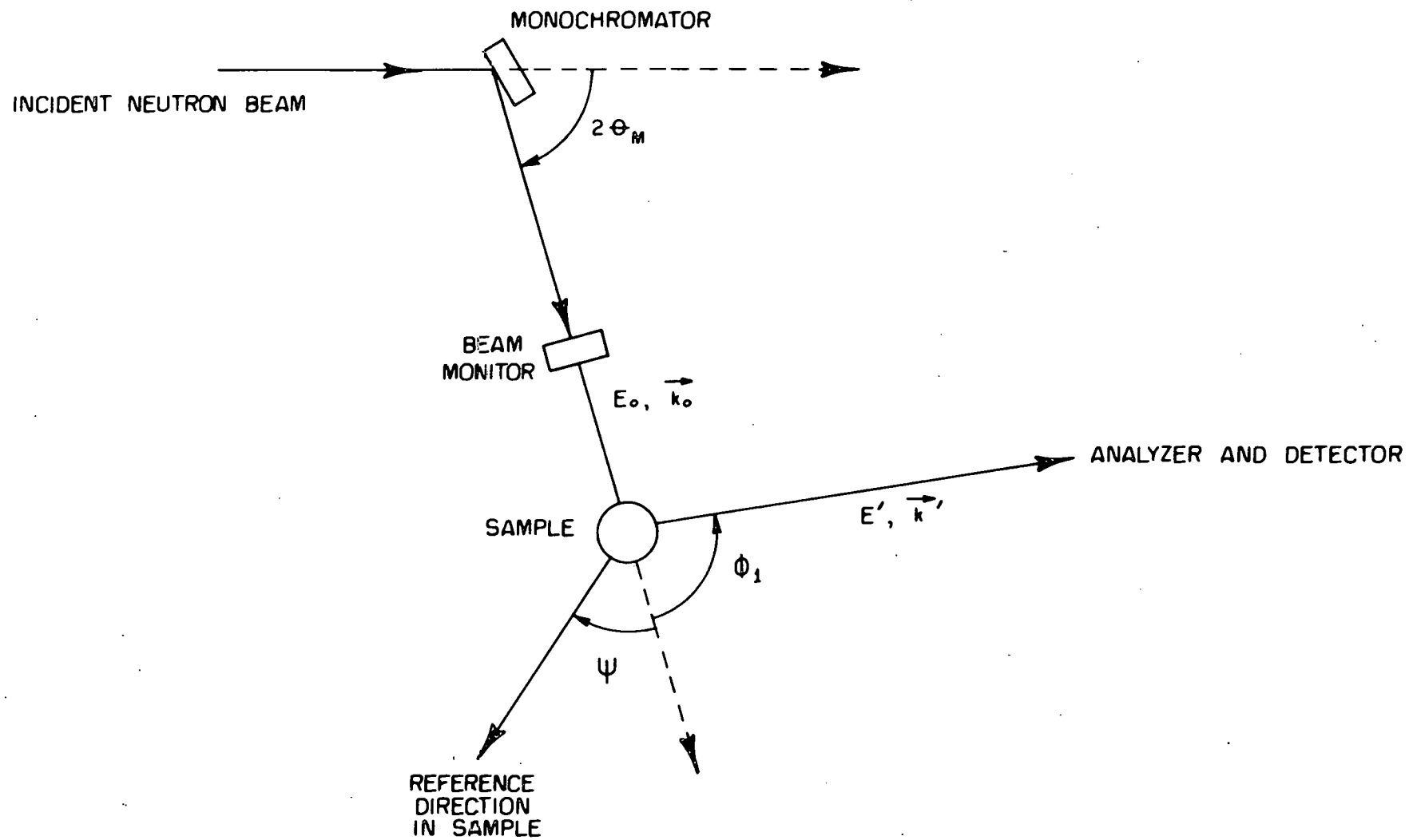


Fig. 3. Angular Representation of Spectrometer Components

At this time, ANGL calculates only the angles used to collect data in the scan mode ($2\theta_M$, ψ , and ϕ_1). ANGL operates in one of four modes (Keyboard Command M1, M2, M3, or M4) depending on predetermined restrictions on the values of E_0 , \vec{k}_0 , E' , and \vec{k}' . Each of these modes as well as the other commands are described in the following sections.

CB[†], Read Lattice Parameters

The command CB is a prerequisite for the CA (calculate angles) command in ANGL. Teletype input to CB consists of the lattice parameters ($|\vec{a}_1|$, $|\vec{a}_2|$, $|\vec{a}_3|$) of the sample in angstroms and γ , the angle between \vec{a}_1 and \vec{a}_2 .

DS[†], Read Monochromator Spacing

DS, also a prerequisite call for CA, requests as input the monochromator spacing, d_M .

XO[†], Choose Psi or Omega

XO allows the experimenter to calculate either angle ψ or ω . At present, ω is not used and ψ is determined by default. This subroutine was incorporated for later use when the experimental system is expanded and need not be called at this time.

Before calling CA to determine the angles, the experimenter calls either M1, M2, M3, or M4. Each of these modes requests different input values depending on the nature of the experiment. CA then calculates angles and other parameters accordingly.

M1[†], Mode 1 Input

Mode one calls for the following input values:

1. l_1 , l_2 , and l_3 , which are components of $\vec{Q} \equiv \vec{k}_0 - \vec{k}'$.

[†]The items designated by the "†" represent Keyboard Commands which, when typed by the user, result in a transfer to subroutines of the same name. These subroutines, in turn, perform the functions described for their respective Keyboard Commands.

2. h , k , and l , which represent the direction of \vec{k}' . $l = 0$ in mode one.

3. ν , which is the frequency.

After calling DS, CB, and ML the experimenter calls CA, which calculates $2\theta_M$, ψ , ϕ_1 , and $|\vec{k}_0|$. CA also calls PA for printing the computed parameters.

M2[†], Mode 2 Input

The following values are input in mode two:

1. l_1, l_2, l_3 .
2. ν .
3. $|\vec{k}_0|$.

In this instance, in addition to finding the angles, CA computes k_x' and k_y' and $|\vec{k}'|$.

M3[†], Mode 3 Input

Input values for mode three are:

1. l_1, l_2, l_3 .
2. ν .
3. h, k, l . $l \neq 0$ in mode three.

CA returns $2\theta_M$, ψ , ϕ_1 , and $|\vec{k}_0|$.

M4[†], Mode 4 Input

Input values are:

1. l_1, l_2, l_3 .
2. ν .
3. $|\vec{k}_0|$.

Output values are $2\theta_M$, ψ , ϕ_1 , k_x' , k_y' , and $|\vec{k}'|$.

CA[†], Calculate Angles

The CA Keyboard Command uses the input values from DS, CB, and M1 (or M2, M3, or M4) to compute the three angles needed for a scanning operation. These angles determine the relative orientations of monochromator, sample, and detector so that neutron distribution about the sample can be ascertained before a data collection period is begun.

CA calls PA which outputs all angular settings.

PA[†], Print Angles

PA, the print angles command, may be called explicitly at any time to verify angular values. This program is normally used after a RZ call (see below) so that the corrected values of the angles may be examined.

At present, angles ϕ_2 , ϕ_3 , and ω are not used for scanning purposes and are not computed by ANGL. PA simply lists these as having a value of zero.

RZ[†], Read Angle Corrections

This Keyboard Command reads an angle correction for each of the six angles, makes the adjustment, and stores the corrected values.

PZ[†], Print Angle Corrections

PZ prints the angle correction factors upon request.

Space Space[†], Stop and Reinitialize

Typing two successive spaces results in an interruption of the executing program segment and a reinitialization of ANGL. This command allows the experimenter to stop calculations at any time and reset all parameters for a new start.

2.2 Equipment Positioning Program

Prior to the collection of time-of-flight data, the experimenter must determine the positions the monochromator, sample, and detectors will assume for the duration of the experiment and then position them accordingly. One program, MAINM, performs both of these functions.

MAINM arrives at the optimum settings for the spectrometer components by collecting sample data in the scan mode. The scan is performed by alternately counting diffracted neutrons and repositioning the motors. The counting period may be either a function of time or of a number of Prescaler Monitor counts during which the diffracted neutrons are collected by only one detector. In this mode, the Time-of-Flight Scaler only counts neutron events versus scattering angles and, therefore, no time channel information is transferred in contrast to the normal data collection. (See Section 1.3.2). The PPG is not enabled and no clock pulses are sent to the Scaler, causing only the detector identification to be gated to the computer. A profile of counting rate versus angle is typed on the teleprinter as the scan progresses.

MAINM, given the current shaft position for each motor, can drive the motors to the desired settings. This positioning is accomplished by a series of Keyboard Commands that allow user communication with the system in the same manner as was described for ANGL (Section 2.1.1).

For a more complete understanding of the motor Drive Assembly and its companion software, the reader is again referred to Setup and Control Routines for a Pulsed Neutron Time-of-Flight Spectrometer.³

2.3 Data Collection Program

The data collection program, COLL, accumulates, sorts, displays, and stores the time-of-flight data. In this mode of operation, the PPG modulates the incident neutron beam and events are counted in any desired combination of the sixteen detectors. COLL consists of a main program which initializes all parameters and sets up the various device interrupt service routines; the input/output programs for the Teletype and DECTape; the interrupt service programs; the data collection and display programs; and the sorting program. The duties performed by these programs are implemented by Keyboard Commands by way of the Keyboard Service Routine, KBSR. As in ANGL, the commands are preceded by a CONTROL S and followed by a carriage return. A list of the COLL user commands is found in Table II.

The loading procedure for COLL is similar to that of ANGL:

```

LOADER
> ← COLL (ALT MODE)
↑ S

```

Before executing the collection program, the experimenter must join cables to the chosen detector input connectors on the front panel of the interface cabinet. He must also set a switch determining the number of detectors to be scanned, thus allowing a proportionally higher count rate per detector (see Section 1.3.2). Since the sorted TOF data are stored on DECTape at the conclusion of an experiment, he must mount a tape on logical unit one. Also stored on this DECTape are the PPG sequence files, one of which is stored in memory before a data-taking period begins.

TABLE II

COLL KEYBOARD COMMANDS

Command	Function
IP	Input Experiment Parameters
OP	Output Data at End of Experiment
CD	Collect and Display Data
ID	Interrupt Data Collection
RD	Resume Data Collection
DP	Select Detector to be Displayed
IT	Input Time
Space Space	Stop and Reinitialize

2.3.1 Initialization Subprograms

When the user responds to the loader's CONTROL S, execution of the main program begins. COLL first clears all device flags and disables the API to avoid any spurious interrupts before the service programs have been initiated. It then calls initialization subroutines for the following six devices: the real-time clock, Interrupt Register, Power Fail recovery facility, Time-of-Flight Scaler, Programmed Pulse Generator, and the Hewlett-Packard display unit. Each of these subroutines sets up a jump to the device service program in the appropriate trap register and presets default values for certain parameters which are essentially invariant during a given experiment.

After enabling the API, COLL prepares the teleprinter to accept Keyboard Commands by loading the starting address of KBSR in location 106. A message is then typed to inform the user that the initialization procedure is complete and that the system is "READY FOR COMMANDS". A ">" signals that the program is in a waiting loop pending a command from the user. After a command has been acted upon and completed, control is always returned to this loop after the ">" ready signal has been typed.

2.3.2 Input/Output Subprograms

Teletype I/O Program, IN

The I/O program for the Teletype, IN, has the following calling sequence:

JMS*	IN
JMP	.+5
.DSA	TYPE
.DSA	NUMBER
.DSA	ARRAY
.DSA	IO

The first calling parameter, TYPE, is set to "0" for floating point data or "1" for integer data. ARRAY represents the address of the data block and NUMBER is the number of array elements. IO equals "0" for input or "1" for output.

A physical data record is terminated by a carriage return and mistakes are corrected by striking the rubout key once for each incorrect character.

IP[†], Input Experiment Parameters

The IP command is usually the first one used after loading COLL and its purpose is to allow the experimenter to input parameters for the coming data collecting period. IP requests the number of detectors to be used and their identification (1-16) labels. It then asks for the six parameters which comprise the PPG status word, packs the status word, and transfers it to the Status Register. (The six parameters are listed in Section 1.3.1.)

The user selects a pseudorandom sequence which has been stored on the DECTape mounted on unit one. The sequence file names are SEQF1 BIN, SEQF2 BIN, etc. and in response to "SEQUENCE FILE IS", the user types a "1" or whatever sequence he desires. After reading the sequence

into a buffer area, IP reverses each word of the sequence because the PPG B Register takes the least significant bit first. An IOT is used to transfer the first word of the code to the A Register and the WC and CA of the code are loaded into locations 26_g and 27_g.

An input value is then requested to signal whether the experimental run period will be a function of time or of the intensity of the neutron beam as determined by the Prescaler. If the experiment is to run for a given time, the user inputs the time in minutes and the real-time clock is prepared to run for that time. If the period is to be determined by the Prescaler, the number of monitor pulses is input.

OP[†], Output Data at End of Experiment

OP is the DECTape output program. At the end of a data collection period, a jump to OP is automatically executed. If the user wishes to terminate an experiment prematurely, he can output the data taken to that point by using the Keyboard Command, OP. The program creates an output file name and writes out three preliminary words containing the number of detectors used in the experiment, the total number of channels used, and the number of channels per sequence bit. After this a block of data consisting of the sequential histograms for the detectors is written. After the file is closed, a message giving the file name is typed and control is returned to the main program where all devices and parameters are reinitialized for the next experiment.

Alternate Output Program, HELP

HELP is a backup output program in the event of an unrecoverable DECTape failure or some types of system failure. This program allows

the user to dump data collected up to the time of the malfunction onto paper tape. The program resides in core throughout a collection period and, if needed, can be started manually from the console by setting switches to the starting address of HELP which is obtained from the load map.*

2.3.3 Interrupt Service Subprograms

Each of the interrupt service routines except the Keyboard Service Routine, KBSR, is entered by way of the API trap address to which the device is assigned. When the WC (which is initially set in COLL) overflows, a device flag is raised causing an interrupt on the appropriate API level and a subsequent jump to the device service routine.

Keyboard Service Routine, KBSR

Entry to the Keyboard Service Routine is gained by typing a CONTROL S. This interrupts the program in progress (unless, of course, the executing program is on a higher API level than the Teletype, which operates at level 3) and puts the computer in a wait state pending a Keyboard Command. KBSR disables the PPG and TOF if they are active to eliminate unwanted interrupts. It then stores the contents of the Accumulator, Link, Limit and Index Registers, and the Program Counter so that the execution of a program can be resumed later at the exact point of interruption. This register storage is necessary because it is

*Actually, the address must be HELP+1 since the first word of every subroutine is reserved for information needed to return control to the calling program.

sometimes desirable to interrupt the data taking routines, make changes, and then resume the data collection. (See the commands, ID and RD.)

When the two-character command is typed, KBSR calls the appropriate subroutine if the command was valid. After the subroutine has executed, control is again returned to the COLL wait loop.

TOF Scaler Service Routine, TOFSR

The Time-of-Flight Scaler Service Routine is entered automatically via API trap address 76_g when one of the data buffers is full. TOFSR resets the WC to -400_g and switches data buffers so that the empty one will receive data after the debreak from TOFSR. A software level interrupt is initiated on API level 4 so that the sorting program will operate at a higher priority than other programs having less important functions, such as displaying the data. The sort program does not, of course, shut out interrupts from the IR, clock, and PPG.

TOFSR clears the TOF overflow flag, clearing the way for future TOF interrupts, and debreaks to the sort program unless a higher level has meanwhile requested service. In this case, the higher device is serviced before the sorting routine is entered.

IR Service Routine, IRSR

The Interrupt Register Service Routine is entered when one or more bits are set in the IR. IRSR determines whether the interrupt was caused by a Lag Error, a Sequence Error, or a Prescaler pulse. (See Section 1.3.3.) If the Prescaler bit was set, a check is made to see if the maximum number of pulses has been reached. If so, a flag is set indicating the end of the experiment, all interface modules are disabled, and the data are stored on DECTape by program OP.

IRSR counts Lag and Sequence Errors and takes no action unless ten or more have occurred. In this case, it types an error message so that the experimenter can decide whether to continue the data collection or abort the experiment.

PPG Service Routine, PPGSR

The PPG Service Routine is entered when all of the pseudorandom sequence has passed through the B Register. The sequence is reinitialized by resetting the WC and the CA of the sequence buffer. After clearing the flag, a debreak to the next highest device requesting service is executed. If none has raised a flag, control returns to the program running when the PPG signalled.

Real-time Clock Service Routine, RTCSR

The Real-Time Clock is set to interrupt every minute and the number of interrupts is compared to the preset experimental run time. At the end of this period, RTCSR sets a flag indicating the end of the experiment, disables the clock and all interface devices, and debreaks to OP for data storage.

If the experiment is not finished, RTCSR resets location 7, enables the clock again, and debreaks.

Power Fail Service Routine, PFSR

The Power Fail Service Routine stores the contents of active registers which will be lost when the system loses power. It is entered when the power low flag is set, indicating a drop in the system line voltage. Before the system stops, PFSR prepares for a

restart and subsequent restoration of the registers by storing a jump to a recovery routine in location 0. When power is restored, program execution resumes in location 0.

2.3.4 Data Collection and Display Programs

CD[†], Collect and Display Data

CD is the subprogram which has control for virtually all the time during an experimental run. It is a background routine which performs the lowest priority chore - that of displaying the incoming TOF data - and hence operates at a lower level than the API and PI.

CD is entered by way of a Keyboard Command after IP has been called to set up all experimental parameters. CD activates the clock or Prescaler, the IR, PPG, and TOF. A loop is then entered which displays the time channels versus count rate for a chosen detector. (See Command DP.) Also included in the loop is a check of the experiment finished flag which is set by RTCSR or IRSR. When the flag is raised, a jump to OP results in the storage of all data taken during the run.

ID[†], Interrupt Data Collection

The ID Keyboard Command causes the data collection process to be suspended without disturbing any of the experimental conditions. ID disables all interface devices and stores registers which will be needed for a restart of the experiment at the point of interruption. The user may make adjustments in the apparatus or may change computer parameters by using the Keyboard Commands. Commands normally used here are IP, OP, IT, or DP. If the user decides to halt the experiment at this time, he can call OP if he wishes to save the data or use the double space command if not.

RD[†], Resume Data Collection

After making the desired adjustments, the user can resume data collection by typing the RD command. RD restores the appropriate registers, enables devices, and jumps to the location interrupted by the ID command.

DP[†], Select Detector to be Displayed

DP is one subroutine commonly called after the data collection has been suspended by the ID command. DP allows the user to select the detector which is being displayed on the oscilloscope. Detector 1 is always shown by default if the DP Keyboard Command has not been used.

IT[†], Input Time

After noting the progress of the experiment, the user may wish to change the length of the data taking period. IT is the Keyboard Command used to input the time factor, which replaces the value input to IP and determines how much longer the experiment will continue after RD is typed.

2.3.5 Sorting Subprogram

The sorting program operates on API level 4 and takes precedence over all others except the device service programs. SORT examines each of the 400 words and uses the detector identification (bits 14-17) and time channel information (bits 2-13) to increment the appropriate location in a large buffer area. This portion of core is now limited to 4230₈ locations. A larger number of detectors, of course, dictates correspondingly fewer time channels since the array size is constant.

2.4 Correlation Program

Modulation of the incident neutron beam by the pseudorandom function completely changes the characteristics of the spectrum that is recorded by the TOF Scaler. Therefore, the modulating function must have characteristics which allow the data as it would normally be measured to be recovered from the smeared TOF spectrum. There is a class of pseudorandom sequences (called pseudorandom because their time distribution approximates that of a random process) which satisfies this condition. Before a proper evaluation of an experiment can be made, a cross correlation of the raw TOF data and the sequence must be computed to retrieve the desired spectrum.

Program CORR performs this cross correlation and displays the corrected data. The program is made up of a main program, which initializes both the display parameters and the Keyboard Service Routine (KBCORR); input/output subroutines; display subroutines; and the correlation subroutine. These subprograms are described in the following paragraphs.

2.4.1 Input/Output Subprograms

DECTAPE I/O Program, RWFILE

RWFILE is a DECTape I/O program which has the following calling sequence:

JMS*	RWFILE
JMP	.+3
.DSA	ADDRESS /Array Address
.DSA	IO /0 for Input, 1 for Output

This subroutine expects to read a file written in the format described

in the section on OP when IO equals zero. Output files from RWFILE are in the same format.

Subroutine IN, described earlier, is used for Teletype I/O.

RE[†], Read Data Files from DEctape

The Keyboard Command, RE, is used to input the raw TOF data file and a corresponding sequence file in preparation for a cross correlation of the two. RE is a prerequisite command for all others in COLL.

WR[†], Write Data on Teletype

WR outputs on the Teletype any elements of the raw data array, the sequence array, or the correlated data array that the experimenter wishes to see. It is called from RE before the correlation process so that the user may scale the raw data if necessary to prevent an overflow during correlation. If the user indicates that he wishes to examine part of one of the arrays, the program requests the detector number and channel number to determine the range of elements to print. WR will also print the identification data stored in the file (see OP) if needed.

2.4.2 Display Subprograms

DP[†], Select Display Parameters

Subroutine DP sets up the display parameters unless the user chooses to accept the default values established by the main program. DP requests the detector to be displayed, upper and lower channels of that detector, and vertical and horizontal scale factors.

SC[†], Display Spectrum on Oscilloscope

SC is the correlated spectrum display program and is called after RE, CO, and DP. The spectrum is shown continuously until the user interrupts SC with another command.

[†] Recall that "+" indicates a keyboard command.

TABLE III

CORR KEYBOARD COMMANDS

Command	Function
RE	Read Data Files
WR	Output Data on Teletype
DP	Select Display Parameters
SC	Display Spectrum
FO	Change Display Scale Factors
PI	Choose Displayed Points Increment
CO	Correlate Raw TOF Data With Sequence
Space Space	Stop and Reinitialize

FO[†], Change Display Scale Factors

The user may wish to change certain display parameters without calling DP (which requires several values). The ones most frequently changed are the scale factors, so a command, FO, was included for this purpose.

PI[†], Choose Displayed Points Increment

The PI command allows the user to limit the number of points on the scope for clarity. For example, he may choose to display every third point in the spectrum.

2.4.3 Correlation Subprogram

CO[†], Correlate Raw TOF Data with Sequence

As pointed out earlier, the spectrum recorded by program COLL bears no resemblance to the desired spectrum. However, it can be recovered by cross correlating the measured spectrum, $Z(t)$, with the pseudorandom sequence, $S(t)$, when $S(t)$ is randomly distributed in time. The function $F(t)$ for time channel I is computed from the following expression:

$$F(I) = \sum_{J=1}^N S(J) \cdot Z(J+I),$$

where N = the number of sequence bits.

A call to subroutine CO produces the correlated function, F , after RE has been used to input S and Z . The correlated data is stored on DECTape.

2.5 File Manipulation Program

Program CALC performs simple manipulations of the data files containing the Z or F functions. It also incorporates the display and output commands described for program CORR. Table IV is a summary of the Keyboard Commands available in CALC.

AD[†], Add Arrays from Two Files

One function of CALC is the consolidation of two or more data files. This is useful when the experimenter has collected data for several short periods under the same experimental conditions and wishes to treat it as if it were a set representative of a longer experiment. AD requires two file names as input. After reading the files from DECTape, control is returned to the wait loop so that the user may examine the files before they are added. The addition is performed by the Keyboard Command, GO. That is, the $F(t)$ (or $Z(t)$, as the case may be) value for each time channel of each detector is added to the corresponding $F_1(t)$ in the second file. The resulting array replaces the original $F(t)$ array in core and then can be examined by using the commands SC and WR. The consolidated array is written on DECTape with a file name of the user's choice. By repeated use of AD and GO, the user can add as many files as necessary.

AV[†], Average Values Within a File

The AV command is used in conjunction with the GO command to average $F_1(t)$ values for selected time channels for each detector. The purpose is to produce better resolution of the spectrum for viewing on the oscilloscope and for performing statistical analyses. AV requests a file name and the number of time channels over which the

averaging will be done. The command, GO, initiates transfer to a subroutine which computes and outputs the array of averaged points. The expression used to average is:

$$F(J) = \sum_{I=J}^{NP+J-1} F_1(I)/NP.$$

AC[†], Add Values Within a File

The AC command is used to add corresponding $F_1(t)$ values for two or more detectors within the same file. AC requests a file name and the detectors (by ID number) to be added. GO is then called to perform the calculations and output the resulting array, $F(t)$.

SU[†], Subtract a Constant

Before calling GO, the experimenter may wish to subtract a constant from each $F_1(t)$ (and $F(t)$, also, in the case where two files are read) to prevent an overflow in the event of high counting rates.

DV[†], Scale Array

DV may be used before GO to scale the data by a constant.

GO[†], Execute Above Functions

The Keyboard Command, GO, initiates the appropriate computations after the arrays have been set up by AD, AV, AC, SU, and DV. GO then calls RWFILE which stores the new file on DECTape.

DP, SC, FO, PI[†], Display Commands

The functions of the display Keyboard Commands are identical to those described for CORR. The double space command is also available.

WR[†], Write Data on Teletype

The WR command is similar to the WR command in CORR. WR may be used to print selected portions of the $F(t)$ and $F_1(t)$ arrays.

TABLE IV

CALC KEYBOARD COMMANDS

Command	Function
AD	Add $F(t)$ Arrays From Two Files
AV	Average $F(t)$ Values Within a File
AC	Add $F(t)$ Values Within a File
SU	Subtract Constant From $F(t)$
DV	Scale $F(t)$ Array
GO	Execute Above Functions
DP	Same as Table III
SC	Same as Table III
FO	Same as Table III
PI	Same as Table III
WR	Write $F(t)$ and $F_1(t)$ Arrays
IN	Output Additional Information
Space Space	Stop and Reinitialize

IN[†], Output Additional Information

Typing IN produces additional information written on the input and output files which is useful in identifying the experimental data recorded in that file. The values listed are the number of detectors used, the total number of time channels, and the number of channels per pseudorandom sequence bit.

2.6 Plotting Program I

The plotting programs were written to provide a permanent record of the cross correlated time-of-flight data. The first program, XY15, produces either graphs on the Complot incremental plotter or histograms on the Teletype. The plots record the scattered neutron counts versus the change in energy of the neutrons for each detector used during an experiment. XY15 also supplies Keyboard Commands DP, SC, FO, PI, and WR for displaying the data or printing it on the Teletype. It is frequently desirable to view the entire spectrum on the scope before choosing the areas to be plotted. Since the plotter is a relatively slow output device, unnecessary portions of the spectrum may be selectively omitted.

RF[†], Read on a Data File

A correlated data file produced by CORR or CALC is read from DEC-tape by program RF. The corresponding command, RF, is the first one used after XY15 is loaded.

WD[†], Select Plot Width

The WD command is optional and need only be called if the user wants the graphs to be something other than ten inches wide. The

TABLE V

XYL5 KEYBOARD COMMANDS

Command	Function
RF	Read a Data File
WD	Select Plot Width (Inches)
HS	Output Plots
HC	Restart HS After Interrupt
WR	Write F(t) Array
DP	Same as Table III
SC	Same as Table III
FO	Same as Table III
PI	Same as Table III
Space Space	Stop and Reinitialize

length of each plot is ten inches and a four inch space separates successive graphs.

HS[†], Output Plots

The HS command produces the execution of subroutine HSFTN1 which makes the necessary computations, scales the data points, and calls the plotting subprograms.

HS requests as input the channel width, the elastic channel, and lattice vectors in order to compute the incident wavelength, the incident wavevector, and the incident energy. After these values are listed, the user selects the channels he wishes to plot, the background factor (if any) he wishes to subtract, and whether he wants Teletype histograms, Complot graphs, or both. The energy changes of the neutrons are calculated for the corresponding range of time channels and are plotted versus the neutron counts. A plot or histogram (or both) is drawn for each detector before control is returned to the waiting loop, pending further commands.

HC[†], Restart HS After Interrupt

The user may interrupt HS if he wishes to use any other command and resume the plotting at a later time on the current detector without having to start over with detector one. For instance, after HS draws the plot for detector one, the user may wish to change the plot width by calling WD or he may wish to view the spectrum by using the display commands before plotting detector two. After calling WD or EC, he may call HC to restart the plotting at the point of interruption.

If the user chooses to skip a detector, he should input zeros when HS requests the "Minimum and Maximum Histogram Limits".

2.7 Plotting Program II

The second plotting program, CONV, converts the scattered neutron counts to an energy scale and plots the scaled data versus the change in energy, as in program XY15. No histogram plots are produced by CONV but in many other respects, it is similar to XY15. Once again, the displaying and printing commands are available. Also present are the WD and RF commands. The chief purpose of CONV is to smooth portions of the converted data and plot the smoothed curve. An option is included for producing plots showing constant steps in energy.

EN[†], Output Plots

Command EN follows the call to RF. EN can produce up to three plots per detector and requires much of the same input called for by HS. The first of the three sections of EN computes the changes in energy for selected time channels and converts the matching scattered neutron count to an energy scale. The user has the option of having the data outputted to the plotter or having it listed in table form on the teleprinter (or both). Output from this section (as well as sections two and three) can be suppressed, if desired. Section two is concerned with smoothing a chosen segment of the curve computed in segment one. Again, the results may be either plotted or printed. The final section provides for finding constant steps of energy and plotting these values versus the corresponding interpolated converted data. Any of the three sections can be skipped by typing "zero" (or a carriage return) for the input parameter requested at the beginning of the section. As in XY15, all calculations and plots for a single detector can be omitted by setting the "Minimum and Maximum Histogram Limits" to zero.

TABLE VI

CONV KEYBOARD COMMANDS

Command	Function
RF	Same as Table V
WD	Same as Table V
WR	Same as Table V
EN	Output Plots
HC	Restart EN
EC	Restart EN
WF	Write a Data File
DP	Same as Table III
SC	Same as Table III
FO	Same as Table III
PI	Same as Table III
Space Space	Same as Table III

EN calls subroutine WF if the user indicates he wishes to save the smoothed data points on a DECTape file.

WF[†], Write a Data File on DECTAPE

The WF command writes a file on DECTape with a file name of the user's choice.

HC[†], Restart EN

The HC command is available for both plotting programs, XY15 and CONV, and was described in Section 2.6. HC restarts program EN after an interruption.

EC[†], Restart EN

Command EC allows the user to select a different segment of the curve to be smoothed. If, during the execution of segment two of program EN, the user notes from the output that the range of smoothed data points should be altered he may call EC. EC will restart EN at the point where the resolution Gaussian width, W_0 , is requested and the smoothing calculations will be repeated.

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APPENDIX A

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APPENDIX A

Table 1

API CHANNEL/PRIORITY ASSIGNMENTS

Channel (Octal)	Trap Address	Device	Priority Level
0	40	Software Channel 0	4
1	41	Software Channel 1	5
2	42	Software Channel 2	6
3	43	Software Channel 3	7
4	44	DECTape	1
5	45	Magtape	1
6	46	Reserved	
7	47	Reserved	
10	50	Paper Tape Reader	2
11	51	Clock Overflow	3
12	52	Power Fail	0
13	53	Parity	0
14	54	Display	2
15	55	Card Reader	2
16	56	Line Printer	2
17	57	A/D	0
20	60	Interprocessor Buffer	3
21	61	Data Link to System 360	3
22	62	Data Phone	2
23	63	DECdisk	1
24	64	DECTape	1
25	65	PPG Overflow	0
32	72	Multi-Station TTY Control	2
33	73	Multi-Station TTY Control	2
34	74	Background Teleprinter	3
35	75	Background Keyboard	3
36	76	TOF Overflow	0
37	77	IR	2

APPENDIX A

Table 2

IOT LIST FOR SPECIAL DEVICES

	<u>Programmed Pulse Generator</u>
705001	Clear PPG Overflow Flag
705002	Spare
705004	Clear PPG
705021	Spare
705022	PPG Output to Accumulator Bit 17 (Diagnostic)
705024	Transfer Bits 0-17 of Sequence to A Register
705041	Spare
705042	Enable PPG
705044	Transfer Status Word to PPG
705061	Spare
705062	Disable PPG
705064	Single-step PPG Through Sequence (Diagnostic)
	<u>Time-of-Flight Scaler</u>
705101	Clear TOF Overflow Flag
705102	Spare
705104	Spare
	<u>Interrupt Register (16 Bits)</u>
705121	Clear IR Flag
705122	Enable IR
705124	Disable IR
705141	Spare
705142	Transfer IR Contents to Accumulator 2-17
705144	Clear IR Bits as Specified by Accumulator 2-17
705161	Spare
705162	Spare
705164	Set All IR Bits (Diagnostic)

Table 2 (Cont'd.)

	<u>Prescaler</u>
705241	Spare
705242	Clear Prescaler
705244	Enable Prescaler
705246	Clear and Enable Prescaler
705262	Disable Prescaler (Does Not Clear)
	<u>Motor Clock Generator</u>
705302	Enable Motor Clock
705304	Disable Motor Clock
	<u>Solenoid</u>
705401	Activate Solenoid
705402	Deactivate Solenoid

APPENDIX A

Table 3

INTERRUPT REGISTER BIT ASSIGNMENTS

IR Bit	Accumulator Bit	Interrupt
16	2	PPG Sequence Error
15	3	PPG Lag Error
14	4	Spare
13	5	Spare
12	6	Spare
11	7	Spare
10	8	Spare
9	9	Spare
8	10	PHI 3 Degree Marker
7	11	PHI 2 Degree Marker
6	12	PHI 1 Degree Marker
5	13	PSI Degree Marker
4	14	OMEGA Degree Marker
3	15	2-THETA-M Degree Marker
2	16	Motor Clock
1	17	Monitor Prescaler

APPENDIX A

Table 4

Motor/Spectrometer Assignments

Motor	Spectrometer Part
2-Theta-M	Monochromator
Omega	Not Used
Psi	Sample
Phi 1	Detector Mount 1 (Adjacent to exit beam)
Phi 2	Detector Mount 2
Phi 3	Detector Mount 3

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APPENDIX B

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APPENDIX B
SAMPLE RUN
PROGRAM ANGL

KM15 V5A

\$LOAD

LOADER V9A

>ANGL

↑S

READY FOR COMMANDS

>

↑S

02

LATTICE PARAMETERS(A1,A2,A3) =

1.

1.

1.

GAMMA =

90.

>

↑S

05

MONOCHROMATOR SPACING (DM) =

1.

>

↑S

03

MODE 3. Q COORDINATES(Q1,L2,L3) =

1.

1.

1.

NU =

516.

DIRECTION OF K. COORDINATES(H,K,L) =

1
1
1

>

↑S
CA

TH, PHI1, PHI2, PHI3, PSI, OMG =

7.850 -4.305 0.000 0.000 59.040 0.000

K0 =

7.305

>

↑S
M4

MODE 4. Q COORDINATES(L1,L2,L3) =

1.
1.
1.

NU =

516.

K0 =

7.3

>

↑S
CA

.013 05

ITM, PHI1, PHI2, PHI3, PSI, OMG =

7.855 -32.321 0.000 0.000 19.482 0.000

K' =

5.216

KX AND KY =

-1.159 5.085

>
TC

KM15 V5A

\$

APPENDIX B
SAMPLE RUN
PROGRAM COLL

KM15 V5A

\$LOAD

LOADER V9A

> COLL

TS

READY FOR COMMANDS

>

TS

IP

NO. OF DETECTORS =

3

DETECTORS ARE

1

2

3

NO. IN DELTA T SEQUENCE =

682

LAST DELTA T IN SEQUENCE =

3

NO. OF CHANNELS/DELTA T =

1

SEQUENCE FILE IS

3

INPUT 0 FOR COUNT VS. TIME. 1 FOR COUNT VS. MONITOR.

0

EXPERIMENT RUNNING TIME (MIN.) =

60

>

TS

CU

TS

ID

>
 TS
 DP

DETECTOR TO BE DISPLAYED

3

LOWEST CHANNEL IS

1

HIGHEST CHANNEL IS

682

VERTICAL ADJUSTMENT FACTOR

1

HORIZONTAL AND VERTICAL SCALE FACTORS ARE

1

1

>
 TS
 IT

INPUT 0 FOR COUNT VS. TIME. 1 FOR COUNT VS. MONITOR.

0

EXPERIMENT RUNNING TIME (MIN.) =

2

>
 TS
 RD

THE HISTOGRAM OUTPUT FILE IS HDT1-L

READY FOR COMMANDS

>
 TC

KM15 V5A

\$

APPENDIX B
SAMPLE RUN
PROGRAM CORR

KM15 V5A

LOAD

LOADER V9A

→ CORR

TS

READY FOR COMMANDS

>

TS

RE

FILE NAME IS

HDT1-J

CALL WR?

Y

OUTPUT F?

N

ADDITIONAL INFORMATION?

Y

NO. OF DETECTORS, TOTAL NO. OF CHANNELS, AND NO.CHANNELS/DELTA T =

3 2046 1

RAW DATA?

Y

DETECTOR, CHANNELS ARE

1

1

5

2767 2791 2743 2854 3099

SEQUENCE?

N

CORRESPONDING SEQUENCE IS

3

Z SCALE FACTOR IS

75

>

↑S
CO

FILE NAME IS
CORREJ

>

↑S
WR

OUTPUT F?

Y
DETECTOR, CHANNELS ARE
1
1
5

6960 6959 6956 6941 6948
ADDITIONAL INFORMATION?
N

>

↑S
DP

DETECTOR TO BE DISPLAYED
1
LOWEST CHANNEL IS
120
HIGHEST CHANNEL IS
230
VERTICAL ADJUSTMENT FACTOR
6940
HORIZONTAL AND VERTICAL SCALE FACTORS ARE
10
1

>

↑S
SC
↑C

KM15 V5A

APPENDIX B

SAMPLE RUN

PROGRAM CALC

KM15 V5A

\$LOAD

LOADER V9A

>CALC,RWFILE

↑SS

READY FOR COMMANDS

>

↑S

AD

FILE NAME IS

FDIXG

FILE NAME IS

FDIXH

>

↑S

SU

SUBTRACT

-500

>

↑S

GO

FILE NAME IS

CORREJ

>

↑S
AC

FILE NAME IS
FDIHXH

NO. OF DETECTORS TO BE ADDED =

2
DETECTORS ARE

1

3

>

↑S
GO

FILE NAME IS
CORREJ

>

↑S
WR

OUTPUT F?
Y
DETECTOR, CHANNELS ARE
1
1
S

13708 13720 13733 13745 13734 13705
F1?

Y
DETECTOR, CHANNELS ARE
1
1
6

7843 7832 7838 7832 7839 7824

>

↑C

KM10 V5A

APPENDIX B

SAMPLE RUN

PROGRAM XY15

KM15 V5A

LOAD

LOADER V9A

>XY15

↑S

READY FOR COMMANDS

>

↑S

RF

FILE NAME IS

ADFG12

>

↑S

HS

CHANNEL WIDTH=

11.765

ELASTIC CHANNEL=

186.6

LATTICE VECTORS=

4.83 4.83

AL1 AND AL2=

193.0 152.3

INCIDENT WAVELENGTH = 0.25152E+01 Å

INCIDENT WAVEVECTOR = 0.39759E+00 (Å)⁻¹

INCIDENT ENERGY = 0.12930E+02 MEV

CHANNELS AND CHANNEL GROUPING (ODD)

LOW	HIGH	GROUP
200	220	1

BACKGROUND CHANNELS=

1 20

INPUT 0 FOR PLOTS, 1 FOR TT OUTPUT, 2 FOR BOTH

DETECTOR 1

BACKGROUND= 17560.

MINIMUM AND MAXIMUM COUNTS =

17578 17911

MINIMUM AND MAXIMUM HISTOGRAM LIMITS =

17570 17900

CRYSTAL AND SCATTERING ANGLES=

200	17671.	3.37	100000000010000
201	17739.	3.56	10000000001000000000100000
202	17766.	3.75	100000000010000000001000000000
203	17793.	3.94	1000000000100000000010000000001000
204	17831.	4.12	1000000000100000000010000000001000000000
205	17849.	4.29	100000000010000000001000000000100000000010
206	17870.	4.46	1000000000100000000010000000001000000000100000
207	17865.	4.63	1000000000100000000010000000001000000000100000
208	17882.	4.79	1000000000100000000010000000001000000000100000
209	17911.	4.94	100000000010000000001000000000100000000010000000001
210	17862.	5.09	10000000001000000000100000000010000000001000
211	17828.	5.24	1000000000100000000010000000001000000000100000000
212	17859.	5.38	1000000000100000000010000000001000000000100000000
213	17837.	5.52	1000000000100000000010000000001000000000100000000
214	17771.	5.65	100000000010000000001000000000
215	17779.	5.78	10000000001000000000100000000010
216	17784.	5.91	10000000001000000000100000000010
217	17697.	6.03	1000000000100000000
218	17578.	6.16	1
219	17613.	6.27	1000000
220	17638.	6.39	1000000000

>

10

KM15 V5A

\$

APPENDIX B
 SAMPLE RUN
 PROGRAM CONV

KM15 V5A

\$A DID2 -4,-5

\$LOAD

LOADER V9A

*-CONV

TS

READY FOR COMMANDS

>

TS

RF

FILE NAME IS
 ADFG12

>

TS

EN

CHANNEL WIDTH=

11.765

ELASTIC CHANNEL=

136.6

D0 AND D1=

193.0 152.3

CHANNELS

LOW

HIGH

200

220

BACKGROUND CHANNELS=

1

20

DETECTOR 1

BACKGROUND= 17560.

MINIMUM AND MAXIMUM COUNTS=

17581

17913

MINIMUM AND MAXIMUM HISTOGRAM LIMITS=

17500 17900

0 - PLOT, 1 - TT OUTPUT, 2 - BOTH, 3 - NEITHER

1

T	S(Q,E)	E
200	17673	3.37
201	17740	3.56
202	17768	3.75
203	17795	3.94
204	17833	4.12
205	17851	4.29
206	17872	4.46
207	17867	4.63
208	17885	4.79
209	17913	4.94
210	17864	5.09
211	17831	5.24
212	17861	5.38
213	17839	5.52
214	17774	5.65
215	17782	5.78
216	17787	5.91
217	17700	6.03
218	17581	6.16
219	17616	6.27
220	17641	6.39

W0=

.5

0 - PLOT, 1 - TT OUTPUT, 2 - BOTH, 3 - NEITHER

1

MINIMUM AND MAXIMUM COUNTS=

17617 17881

MINIMUM AND MAXIMUM LIMITS=

17617 17881

T	SP(Q,E)	E
200	17707	3.37
201	17736	3.56
202	17768	3.75
203	17798	3.94
204	17826	4.12
205	17848	4.29
206	17863	4.46
207	17874	4.63
208	17881	4.79
209	17879	4.94
210	17867	5.09
211	17852	5.24
212	17837	5.38
213	17818	5.52
214	17795	5.65
215	17767	5.78
216	17732	5.91
217	17691	6.03
218	17656	6.16
219	17632	6.27
220	17617	6.39

DELTA E AND E0=

.25

0.

WRITE FILE

N

0 - PLOT, 1 - TT OUTPUT, 2 - BOTH, 3 - NEITHER

1

SP(Q,E)	E(EVEN INTERVALS)
17737	3.37
17744	3.62
17786	3.87
17825	4.12
17854	4.37
17873	4.62
17879	4.87
17864	5.12
17838	5.37
17800	5.62
17743	5.87
17667	6.12
17619	6.37

>

↑C

KM15 V5A

\$

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