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PROGRAM FOR THE LOCATION OF FOURIER PEAK CENTERS

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Metallurgy Divison

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ABSTRACT

The location of maxima on Fourier (or Patterson) maps is accomplished with a computer program, written in FORTRAN, for obtaining the peak location and height from 27 surrounding points in the 3-dimensional Fourier and from 9 points for a 2-dimensional case.

INTRODUCTION

Although the location of the peak or maxima on Fourier maps can be estimated by contour lines and by interpolation, this method has limited accuracy. As a result, analytical extrapolation techniques, such as that of Booth,[1] have been worked out. Later, Schoemaker et al.,[2] described the least-squares fitting of 27 points about the maximum on a three-dimensional Fourier summation to a ten-parameter Gaussian function. This scheme has since been used in computer programs such as that of Ibers,[3] Bryden,[4] and the presently described program. Basically, all of these are very similar and have been written in FORTRAN. The Ibers program makes use of the 27 points for 3-dimensional peaks whereas the Bryden program makes use of the 19 points closest to the maximum as suggested by Donahue and Trueblood.[5] The Bryden program also includes a system for peak location on a 2-dimensional Fourier based on 9 points about the maximum. The present program, MET-146, uses 27 points for the 3-dimensional program and 9 points for the 2-dimensional cases. It eliminates the need for input to be in a specific order, allows any number of three- or two-dimensional cases to be run simultaneously, and gives more information in the output.

DISCUSSION

The program, which has been written in FORTRAN, requires only the intensity, or ρ values, at the points around the maximum together with an indication of whether the problem is 3- or 2-dimensional.

In the 3-dimensional case, 27 points in a 3 x 3 x 3 rectangular parallelepiped as close as possible to the peak maximum are fitted by least squares to the following ten-parameter Gaussian function ρ:

$$\ln \rho = p - \frac{r}{2} x^2 - \frac{s}{2} y^2 - \frac{t}{2} z^2 + ux + vy + wz + lyz + mxz + nxy \quad ,$$

where x, y, and z are the coordinates of the 27 observed density values. In order to facilitate computation, it is convenient to take the central point of the 27 as the origin (0,0,0) and to describe the other 26 values in terms of this origin rather than in terms of the map origin. Thus, all coordinates are restricted to values of ± 1 or 0. The coordinate of the maximum density, when found, is then converted back to the map coordinate system (X,Y,Z). An analogous procedure to that described above is followed for two-dimensional cases.

By designating the number of cases on the input cards, one may include the data for 1 to 11 cases on the same input set of cards. Three- and 2-dimensional cases may not be mixed on the same input set of cards (a set is considered to be 27 or 9 cards); however, any number of sets may follow each other without again feeding in the program deck.

In 2-dimensional problems it is necessary that all cases, if they are to be included on the same set of data cards, must refer to the same orientation in space, that is, must have a common zone axis.

The input data also calls for the size of the Fourier map intervals, that is, 1/60th, 1/120th, etc., which are not necessarily the same in each direction. This information is included as a decimal part according to the following scheme:

	DX, DY or DZ
1/240 =	0.004167
1/120 =	0.008333
1/60 =	0.016667
1/30 =	0.033333

The output data include certain parameters obtained in the solution of the problem which assist in detecting errors. A print-out of the input ρ values, the calculated ρ values, and the differences are also printed out. In this way it is easy to judge the fit obtained from the least-squares solution.

The next part of the output gives the peak location in terms of the map coordinates and in terms of the decimal parts of the unit-cell lengths.

When the present program, known as MET-146, was written in its original form, the Ibers and Bryden programs had not been obtained; but when these programs became available a comparison was made of the results of the MET-146 program with those of the other two programs. The same 3-dimensional data were used as input for each of the three programs. The results are shown in Table I together with the values obtained from the Booth analytical extrapolation method.

Table I

SUMMARY OF FOURIER PEAK RESULTS* OBTAINED BY SEVERAL DIFFERENT METHODS

Peak Designation		Analytical Extrapolation		Ibers Program		Bryden Program		MET-146	
N-2	x=	26.93	0.22442	27.67	0.2306	27.67	0.23056	27.67	0.23061
	y=	12.08	0.10067	12.11	0.1009	12.11	0.10088	12.10	0.10087
	z=	10.21	0.17017	10.33	0.1721	10.33	0.17213	10.32	0.17214
	Peak Ht.			2356		2357		2356	
O-3	x=	16.37	0.13642	15.44	0.1287	15.43	0.12855	15.45	0.12874
	y=	13.04	0.10867	12.95	0.1079	12.95	0.10788	12.94	0.10786
	z=	9.13	0.15217	8.70	0.1450	8.67	0.14457	8.70	0.14503
	Peak Ht.			738.5		741		739	
N-4	x=			25.99	0.2166	25.99	0.21661	25.99	0.21661
	y=			47.71	0.3976	47.72	0.39764	47.72	0.39764
	z=			10.34	0.1723	10.34	0.17228	10.34	0.17226
	Peak Ht.			6521.9		6531		6522	
O-4	x=			37.79	0.3149	37.78	0.31483	37.79	0.31493
	y=			17.52	0.1460	17.53	0.14608	17.52	0.14602
	z=			18.24	0.3040	18.24	0.30398	18.24	0.30398
	Peak Ht.			2138.3		2143		2138	

*The first column of each result is the map coordinate and the second column is decimal part of the unit cell. Only MET-146 prints out the two results.

INPUT CARDS

Card	Format	Columns	Contents
1	72H	2-72	Title (first column blank)
2	3E12.8	1-36	DX, DY, and DZ = decimal equivalent length for one map unit in the three respective directions used to transform results to the decimal part of the unit cell.
		1-12	DX, decimal in column 4
		13-24	DY, decimal in column 16
		25-36	DZ, decimal in column 18
	I6	37-42	K = number of cases (or sets or data) being combined in this group ($1 \leq K \leq 11$).
	I6	43-48	N = number of data points (N = 27 or 9).
3	6X,11F6.0	7-72	Map coordinates, in X direction, of the points chosen as the origin (0,0,0) of the 27-point set. (K number of values.)
		7-12	X coordinate, 1st case.
		13-18 etc.	X coordinate, 2nd case.
4	6X,11F6.0	7-72	Map coordinates, in Y direction, of the points chosen as the origin (0,0,0) of the 27-point set. (K number of values.)
		7-12 etc.	Y coordinate, 1st case.
5	6X,11F6.0	7-72	Map coordinates, in Z direction, of the points chosen as the origin (0,0,0) of the 27-point set. (K number of values.)
		7-12 etc.	Z coordinate, 1st case.
6	6X,11A6	7-72	Atom identifications (K number of atoms).
		7-12	Identification for case No. 1 such as 0-3.

Card	Format	Columns	Contents
7 through N (27 or 9)+6	3I2	1-6	(a) x,y,z coordinate values using all necessary combinations of the integers -1, 0, +1.
	11F6.0	7-72	(b) Values of ρ for K cases. (The order of the coordinates is immaterial as long as 000 is first.)
		7-12 etc.	ρ value, 1st case.

OUTPUT INFORMATION

(a) Program identification

(b) Title

(c) Atom identification

(d) Values of Gaussian coefficients

(e) Values of x, y, z, ρ_{obs}, ρ_{calc}, $\rho_{obs}-\rho_{calc}$ for each of the N points

(f) Coordinates of peak corrected to map coordinates

(g) Coordinates of peak corrected to the decimal part of the unit cell

(h) Peak height at above coordinates

CARD DECK ARRANGEMENT

IBM-704

Peak Location binary program deck

Card 1. (Title card)

Card 2. (DX, DY, DZ)

Card 3. (Map Coordinate of X of origin)

Card 4. (Map Coordinate of Y of origin)

Card 5. (Map Coordinate of Z of origin)

Card 6. (Atom identification)

Card 7-33. (x,y,z and ρ_{obs} values, 3-dimensional)

or Card 7-15. (x,y,z and ρ_{obs} values, 2-dimensional)

Note 1: More than one set of computations can be made by using additional data cards 1, 2, 3, etc, in sequence. These cards should be placed after the initial set of data cards. The last set of data cards should always be followed by 2 blank cards.

RUNNING TIME

Less than one minute per case.

1552/Met 146
704 PROGRAM

Programmer: F. Clark *Date*: 2/15/63

GENERAL OPERATING INSTRUCTIONS

	USED	NOT USED
DRUM:	[ ]	[x]
UF SWITCH:	[x]	[ ]

READER: 72 x 72 Board

PUNCH: Not Used

PRINTER: Not Used

SENSE SWITCH SETTINGS: None

TAPES:

Input: Tape No. 7
FORTRAN Library Tape No. 1

Scratch:

Output - Printed: Tape No. 6
- Punched

To Be Saved: None

Rewound by Program Prior to Calculation None After None

Manual EOF Needed Tape No. 6

TIME BEFORE OUTPUT: 10 sec/case

NORMAL RUNNING TIME: 1 min/case

RUN NO LONGER THAN: 2 min/case

RUNNING PROCEDURE: *(Indicate both regular and restart)*

(1) Mount and Ready tape No. 6 for Output
(2) Mount and Ready tape No. 7 for Input
(3) FORTRAN Library tape on unit No. 1
(4) CLEAR and LOAD CARDS
(5) At HPR 0,1 (E.O.F. on input tape) problem is finished. Write E.O.F. on tape No. 6. Remove and print off-line on program control

STOPS (OCTAL): FORTRAN error stops

TEST PROBLEM

The input and output data for two different peaks, N2 and O3, are included to afford an opportunity to check the program out. Figure 1 shows the data sheet used for punching the necessary IBM cards. Figure 2 is a direct copy of the output sheets obtained for these peaks. The title and the input information are printed out together with the ρ_{calc} and ρ difference. The values obtained for the peak in terms of map coordinates are given followed by the conversions of these values to decimal parts of the unit cell.

704 INPUT DATA

FORM 11

Figure 1. MET-146 704 DATA SHEETS-TEST PROBLEM

COST CODE 1552

PROGRAM MET-146 PROBLEM Ru Cpd ORIGINATOR Mueller DATE 2/22/63 PAGE 1 OF 2

1552 MET 146 MUELLER FOURIER PEAK LOCATION TEST PROBLEM 2/22/63

	.0083333		.0083333		.0166667	2	27
	27	16					
	12	13					
	10	9					
	N-2	0-3					
0 0 0	2294	727					
-1 0 -1	1908	717					
-1 0 0	1995	709					
-1 0 1	1604	571					
0 0 -1	1987	658					
0 0 1	2064	659					
1 0 -1	1778	498					
1 0 0	2267	637					
1 0 1	2255	650					
-1 -1 -1	1648	653					
-1 -1 0	1753	678					
-1 -1 1	1429	578					
0 -1 -1	1690	582					
0 -1 0	1989	675					

AMD-9 (9-60)

704 INPUT DATA

FORM II

COST CODE 1552

Figure 1 (Continued)

PROGRAM MET-146 PROBLEM Ru Cpd ORIGINATOR Mueller DATE 2/22/63 PAGE 2 OF 2

0 -1 1	1815	644
1 -1 -1	1493	416
1 -1 0	1944	566
1 -1 1	1965	616
-1 1 -1	1729	671
-1 1 0	1780	624
-1 1 1	1388	469
0 1 -1	1828	641
0 1 0	2080	665
0 1 1	1826	563
1 1 -1	1658	505
1 1 0	2092	599
1 1 1	2042	571

AMD-9 (9-60)

Figure 2. MET-146 704 OUTPUT SHEETS-TEST PROBLEM

TITLE 1552/MET 146, CODE E2. MACHINE 704F

1552 MET 146 MUELLER FOURIER PEAK LOCATION TEST PROBLEM 2/22/63

N-2

P	R	S	T	U
7.74079734	0.15450858	0.24455260	0.25866698	0.06815001

V	W	L	M	N
0.02111454	0.01628578	-0.01799421	0.10470875	0.01520672

X	Y	Z	RHO	RHO CALC	DELTA RHO
0	0	0	2294.	2300.305725	-6.305725
-1	0	-1	1908.	1909.282181	-1.282181
-1	0	0	1995.	1989.011597	5.988403
-1	0	1	1604.	1599.804504	4.195496
0	0	-1	1987.	1988.584030	-1.584030
0	0	1	2064.	2054.421661	9.578339
1	0	-1	1778.	1774.661774	3.338226
1	0	0	2267.	2279.458221	-12.458221
1	0	1	2255.	2260.529022	-5.529022
-1	-1	-1	1648.	1649.626846	-1.626846
-1	-1	0	1753.	1749.716461	3.283539
-1	-1	1	1429.	1432.887344	-3.887344
0	-1	-1	1690.	1692.214279	-2.214279
0	-1	0	1989.	1993.020416	-4.020416
0	-1	1	1815.	1812.301865	2.698135
1	-1	-1	1493.	1487.383026	5.616974
1	-1	0	1944.	1945.152405	-1.152405
1	-1	1	1965.	1964.024277	0.975723
-1	1	-1	1729.	1730.400879	-1.400879
-1	1	0	1780.	1770.513153	9.486847
-1	1	1	1388.	1398.665909	-10.665909
0	1	-1	1828.	1829.888947	-1.888947
0	1	0	2080.	2078.986115	1.013885
0	1	1	1826.	1823.647308	2.352692
1	1	-1	1658.	1658.061249	-0.061249
1	1	0	2092.	2091.711792	0.288208
1	1	1	2042.	2037.349472	4.650528

X,Y,Z, VALUES CORRECTED TO MAP COORDINATES

27.67396975	12.10407376	10.32854438

X,Y,Z, MAP COORDINATES CORRECTED TO UNIT CELL COORDINATES

0.23061632	0.10086723	0.17214244

PEAK HEIGHT

2356.16809082

O-3

P	R	S	T	U
6.59479624	0.17571480	0.17094293	0.20883845	-0.05767016

V	W	L	M	N
-0.00793773	0.00260586	-0.06140602	0.12413509	0.03662156

X	Y	Z	RHO	RHO CALC	DELTA RHO
0	0	0	727.	731.279861	-4.279861
-1	0	-1	717.	721.779022	-4.779022
-1	0	0	709.	709.534401	-0.534401
-1	0	1	571.	566.037643	4.962357
0	0	-1	658.	657.057281	0.942719
0	0	1	659.	660.490616	-1.490616
1	0	-1	498.	501.753342	-3.753342
1	0	0	637.	632.239792	4.760208
1	0	1	650.	646.511192	3.488808
-1	-1	-1	653.	651.580406	1.419594
-1	-1	0	678.	681.091576	-3.091576
-1	-1	1	578.	577.757591	0.242409
0	-1	-1	582.	571.824120	10.175880
0	-1	0	675.	676.723320	-1.723320
0	-1	1	644.	649.923851	-5.923851
1	-1	-1	416.	420.964031	-4.964031
1	-1	0	566.	564.033424	1.966576
1	-1	1	616.	613.292076	2.707924
-1	1	-1	671.	673.908508	-2.908508
-1	1	0	624.	623.019791	0.980209
-1	1	1	469.	467.417976	1.582024
0	1	-1	641.	636.362289	4.637711
0	1	0	665.	666.064857	-1.064857
0	1	1	563.	565.758728	-2.758728
1	1	-1	505.	504.075974	0.924026
1	1	0	599.	597.336777	1.663223
1	1	1	571.	574.440666	-3.440666

X,Y,Z, VALUES CORRECTED TO MAP COORDINATES

15.44933510	12.94263244	8.70202684

X,Y,Z, MAP COORDINATES CORRECTED TO UNIT CELL COORDINATES

0.12874440	0.10785522	0.14503381

PEAK HEIGHT

738.51707458

SOURCE DECK LISTING

```
C                  PROBLEM 1552/MET 146  FRED CLARK  8/62
C          ATOMIC CENTER LOCATION FOR TWO AND THREE DIMENSIONAL
C      FOURIER MAPS
C           THIS PROBLEM INVOLVES THE LEAST SQUARES FITTING OF A TEN PAR
C      AMETER GAUSSIAN FUNCTION BY THE METHOD OF LEAST SQUARES.
C      THE FUNCTION IS  RHO=EXP(P-R/2*X**2-S/2*Y**2-T/2*Z**2
C           +U*X+V*Y+W*Z+L*Y*Z+M*X*Z+N*X*Y.............
       DIMENSION X(27),Y(27),Z(27),SUM(20,1),RHO(11,27),
      XA(20,20),B(20,1),R(10,3),REAL(3),CUE(27),CCUE(27),DELTA(27),AA(11)
      X,KX(27),KY(27),KZ(27)
  100  FORMAT(42H1TITLE 1552/MET 146, CODE E2. MACHINE 704F//)
  102  FORMAT(/1H04X,1HX5X,1HY5X,1HZ8X,3HRHO6X,8HRHO CALC5X,
     X9HDELTA RHO//)
  104  FORMAT(43H0X,Y,Z, VALUES CORRECTED TO MAP COORDINATES)
  105  FORMAT(6X,11F6.0)
  106  FORMAT(3F2.0,11F6.0)
  108  FORMAT(1H014X,1HP11X,1HR11X,1HS11X,1HT11X,1HU)
  999  FORMAT(7X,F15.8)
  109  FORMAT(1H014X,1HV11X,1HW11X,1HL11X,1HM11X,1HN)
  110  FORMAT(8X,6F12.8)
  111  FORMAT(3F20.8)
  112  FORMAT(1H014X,1HP11X,1HS11X,1HT11X,1HV11X,1HW11X,1HL)
  113  FORMAT(1H014X,1HP11X,1HR11X,1HT11X,1HU11X,1HW11X,1HM)
  114  FORMAT(1H014X,1HP11X,1HR11X,1HS11X,1HU11X,1HV11X,1HN)
  115  FORMAT(72H
     X                )
  116  FORMAT(12H0PEAK HEIGHT)
  117  FORMAT(3I6,F12.0,3X,2F12.6)
  118  FORMAT(1H0,57HX,Y,Z, MAP COCRDINATES CORRECTED TO UNIT CELL COORDI
     1NATES)
  119  FORMAT(6X,11A6)
  121  FORMAT(1H0,A6)
  122  FORMAT(1H1)
  126  FORMAT(3E12.8,2I6)
    1  READ INPUT TAPE 7,115
  127  READ INPUT TAPE 7,126,SFX,SFY,SFZ,K,N
       READ INPUT TAPE 7,105,(R(I,1),I=1,K)
       READ INPUT TAPE 7,105,(R(I,2),I=1,K)
       READ INPUT TAPE 7,105,(R(I,3),I=1,K)
       READ INPUT TAPE 7,119,(AA(I),I=1,K)
       WRITE OUTPUT TAPE 6,100
       WRITE OUTPUT TAPE 6,115
       DO 128 J=1,N
  128  READ INPUT TAPE 7,106,X(J),Y(J),Z(J),(RHO(I,J),I=1,K)
       II=0
       IF(N-9)3,2,3
    2  TOT1 = 0.
       DO 4 I=1,N
    4  TOT1 = TOT1 + ABSF(X(I))
       M = 1
       IF(TOT1)5,20,5
    5  TOT2 = 0.
       DO 6 I=1,N
    6  TOT2 = TOT2 + ABSF(Y(I))
```

```
      M = 2
      IF(TOT2)7,20,7
    7 TOT3 = 0.
      DO 8 I=1,N
    8 TOT3 = TOT3 + ABSF(Z(I))
      M = 3
      GO TO 20
    3 DO 9 I=1,20
S   9 STZ SUM(I,1)
C                          PROBLEM IS THREE DIMENSIONAL
      II=II+1
      WRITE OUTPUT TAPE 6,121,AA(II)
      DO 10 I=1,N
      CUE(I)=LOGF(RHO(II,I))
      SUM(1,1) = SUM(1,1) + CUE(I)
      SUM(2,1) = SUM(2,1)+0.5*X(I)**2*CUE(I)
      SUM(3,1) = SUM(3,1) + 0.5*Y(I)**2*CUE(I)
      SUM(4,1) = SUM(4,1) + 0.5*Z(I)**2*CUE(I)
      SUM(5,1) = SUM(5,1) + X(I)*CUE(I)
      SUM(6,1) = SUM(6,1) + Y(I)*CUE(I)
      SUM(7,1) = SUM(7,1) + Z(I)*CUE(I)
      SUM(8,1) = SUM(8,1) + Y(I)*Z(I)*CUE(I)
      SUM(9,1) = SUM(9,1) + X(I)*Z(I)*CUE(I)
   10 SUM(10,1) = SUM(10,1) + X(I)*Y(I)*CUE(I)
      DO 11 I=1,20
      DO 11 J=1,20
S  11 STZ A(I,J)
      A(1,1) = 27.
      A(2,1) = 9.
      A(3,1) = 9.
      A(4,1) = 9.
      A(1,2) = -9.
      A(2,2) = -4.5
      A(3,2) = -3.
      A(4,2) = -3.
      A(1,3) = -9.
      A(2,3) = -3.
      A(3,3) = -4.5
      A(4,3) = -3.
      A(1,4) = -9.
      A(2,4) = -3.
      A(3,4) = -3.
      A(4,4) = -4.5
      A(5,5) = 18.
      A(6,6) = 18.
      A(7,7) = 18.
      A(8,8) = 12.
      A(9,9) = 12.
      A(10,10) = 12.
      CALL MATINV(A,10,SUM,1,ANY)
      DO 15 I=1,20
      DO 15 J=1,20
S  15 STZ A(I,J)
      A(1,1) = SUM(2,1)
      A(2,1) = SUM(10,1)
      A(3,1) = SUM(9,1)
      A(1,2) = -SUM(10,1)
      A(2,2) = -SUM(3,1)
      A(3,2) = SUM(8,1)
      A(1,3) = -SUM(9,1)
```

```
      A(2,3) = SUM(8,1)
      A(3,3) = -SUM(4,1)
      DO 16 I=1,20
S  16 STZ B(I,1)
      B(1,1) = SUM(5,1)
      B(2,1) = -SUM(6,1)
      B(3,1) = -SUM(7,1)
      CALL MATINV (A,3,B,1,ANY)
      L = 4
      C = CUE(1)-0.5*SUM(2,1)*B(1,1)**2-0.5*SUM(3,1)*B(2,1)**2-0.5*
     XSUM(4,1)*B(3,1)**2+SUM(5,1)*B(1,1)+SUM(6,1)*B(2,1)+SUM(7,1)*B(3,1)
     X+SUM(8,1)*B(2,1)*B(3,1)+SUM(9,1)*B(1,1)*B(3,1)+SUM(10,1)*B(1,1)
     X*B(2,1)
      PH=EXPF(C)
      DO 129 I=1,N
      CCUE(I)=SUM(1,1)-.5*SUM(2,1)*X(I)**2-.5*SUM(3,1)*Y(I)**2-.5*SUM
     X(4,1)*Z(I)**2+SUM(5,1)*X(I)+SUM(6,1)*Y(I)+SUM(7,1)*Z(I)+SUM(8,1)*Y
     X(I)*Z(I)+SUM(9,1)*X(I)*Z(I)+SUM(10,1)*Y(I)*X(I)
      CCUE(I)=EXPF(CCUE(I))
 129  DELTA(I)=RHO(II,I)-CCUE(I)
  50  REAL(1)=B(1,1)+R(II,1)
      REAL(2)=B(2,1)+R(II,2)
      REAL(3)=B(3,1)+R(II,3)
      GO TO (80,81,82,83),L
  83  CONTINUE
      WRITE OUTPUT TAPE 6,108
      WRITE OUTPUT TAPE 6,110,(SUM(I,1),I=1,5)
      WRITE OUTPUT TAPE 6,109
      WRITE OUTPUT TAPE 6, 110, (SUM(I,1), I=6,10)
  90  WRITE OUTPUT TAPE 6,102
      DO 91 I = 1,N
      KX(I) = X(I)
      KY(I) = Y(I)
  91  KZ(I) = Z(I)
      WRITE OUTPUT TAPE 6, 117, (KX(I),KY(I),KZ(I),RHO(II,I),CCUE(I),
     XDELTA(I),I=1,N)
      WRITE OUTPUT TAPE 6,104
      WRITE OUTPUT TAPE 6,111,(REAL(I),I=1,3)
      REAL(1)=REAL(1)*SFX
      REAL(2)=REAL(2)*SFY
      REAL(3)=REAL(3)*SFZ
      WRITE OUTPUT TAPE 6,118
      WRITE OUTPUT TAPE 6,111,(REAL(I),I=1,3)
      WRITE OUTPUT TAPE 6,116
      WRITEOUTPUTTAPE6,999,PH
      WRITE OUTPUT TAPE 6,122
      IF(II-K)39,1,39
  39  IF(N-9)3,20,3
  20  DO 21 I=1,20
      DO 21 J=1,20
S  21 STZ A(I,J)
C         PROBLEM IS TWO DIMENSIONAL
      A(1,1) = 9.
      A(2,1) = 3.
      A(3,1) = 3.
      A(1,2) = -3.
      A(2,2) = -1.5
      A(3,2) = -1.
      A(1,3) = -3.
      A(2,3) = -1.
```

```
      A(3,3) = -1.5
      A(4,4) = 6.
      A(5,5) = 6.
      A(6,6) = 4.
      II=II+1
      WRITE OUTPUT TAPE 6,121,AA(II)
      DO 22 I=1,N
S  22 STZ SUM(I,1)
      DO 69 I=1,20
S  69 STZ B(I,1)
      GO TO (23,24,25),M
   23 DO 26 I=1,N
C        TWO DIMENSIONAL IN Y AND Z
      CUE(I)=LOGF(RHO(II,I))
      SUM(1,1) = SUM(1,1)+CUE(I)
      SUM(2,1) = SUM(2,1)+0.5*Y(I)**2*CUE(I)
      SUM(3,1) = SUM(3,1)+0.5*Z(I)**2*CUE(I)
      SUM(4,1) = SUM(4,1)+Y(I)*CUE(I)
      SUM(5,1) = SUM(5,1)+Z(I)*CUE(I)
   26 SUM(6,1) = SUM(6,1)+Y(I)*Z(I)*CUE(I)
      CALL MATINV(A,6,SUM,1,ANY)
      B(1,1) = 0.
      B(2,1) = -(SUM(4,1)*SUM(3,1)+SUM(6,1)*SUM(5,1))/(SUM(6,1)**2-
     XSUM(2,1)*SUM(3,1))
      B(3,1) = -(SUM(2,1)*SUM(5,1)+SUM(4,1)*SUM(6,1))/(SUM(6,1)**2-
     XSUM(2,1)*SUM(3,1))
      C = CUE(1)-0.5*SUM(2,1)*B(2,1)**2-0.5*SUM(3,1)*B(3,1)**2+
     XSUM(4,1)*B(2,1)+SUM(5,1)*B(3,1)+SUM(6,1)*B(2,1)*B(3,1)
      PH=EXPF(C)
      DO 130 I=1,N
      CCUE(I)=SUM(1,1)-.5*SUM(2,1)*Y(I)**2-.5*SUM(3,1)*Z(I)**2+SUM(4,1)
     X*Y(I)+SUM(5,1)*Z(I)+SUM(6,1)*Y(I)*Z(I)
      CCUE(I)=EXPF(CCUE(I))
  130 DELTA(I)=RHO(II,I)-CCUE(I)
      L = 1
      GO TO 50
   80 WRITE OUTPUT TAPE 6,112
      WRITE OUTPUT TAPE 6,110,(SUM(I,1),I=1,6)
      GO TO 90
   24 DO 33 I=1,N
C                        TWO DIMENSIONAL IN X AND Z
      CUE(I)=LOGF(RHO(II,I))
      SUM(1,1) = SUM(1,1)+CUE(I)
      SUM(2,1) = SUM(2,1)+0.5*X(I)**2*CUE(I)
      SUM(3,1) = SUM(3,1)+0.5*Z(I)**2*CUE(I)
      SUM(4,1) = SUM(4,1)+X(I)*CUE(I)
      SUM(5,1) = SUM(5,1)+Z(I)*CUE(I)
   33 SUM(6,1) = SUM(6,1)+X(I)*Z(I)*CUE(I)
      CALL MATINV(A,6,SUM,1,ANY)
      B(1,1) = -(SUM(5,1)*SUM(6,1)+SUM(3,1)*SUM(4,1))/(SUM(6,1)**2-
     XSUM(3,1)*SUM(2,1))
      B(2,1) = 0.
      B(3,1) = -(SUM(5,1)*SUM(2,1)+SUM(6,1)*SUM(4,1))/(SUM(6,1)**2-
     XSUM(3,1)*SUM(2,1))
      C = CUE(1)-0.5*SUM(2,1)*B(1,1)**2-0.5*SUM(3,1)*B(3,1)**2+
     XSUM(4,1)*B(1,1)+SUM(5,1)*B(3,1)+SUM(6,1)*B(1,1)*B(3,1)
      PH=EXPF(C)
      DO 131 I=1,N
      CCUE(I)=SUM(1,1)-.5*SUM(2,1)*X(I)**2-.5*SUM(3,1)*Z(I)**2+SUM(4,1)
     X*X(I)+SUM(5,1)*Z(I)+SUM(6,1)*X(I)*Z(I)
```

```
      CCUE(I)=EXPF(CCUE(I))
  131 DELTA(I)=RHO(II,I)-CCUE(I)
      L = 2
      GO TO 50
   81 WRITE OUTPUT TAPE 6,113
      WRITE OUTPUT TAPE 6,110,(SUM(I,1),I=1,6)
      GO TO 90
   25 DO 35 I=1,N
C        TWO DIMENSIONAL IN X AND Y
      CUE(I)=LOGF(RHO(II,I))
      SUM(1,1) = SUM(1,1)+CUE(I)
      SUM(2,1) = SUM(2,1)+0.5*X(I)**2*CUE(I)
      SUM(3,1) = SUM(3,1)+0.5*Y(I)**2*CUE(I)
      SUM(4,1) = SUM(4,1)+X(I)*CUE(I)
      SUM(5,1) = SUM(5,1)+Y(I)*CUE(I)
   35 SUM(6,1) = SUM(6,1)+X(I)*Y(I)*CUE(I)
      CALL MATINV(A,6,SUM,1,ANY)
      B(1,1) = -(SUM(4,1)*SUM(3,1)+SUM(6,1)*SUM(5,1))/(SUM(6,1)**2-
     XSUM(3,1)*SUM(2,1))
      B(2,1) = -(SUM(6,1)*SUM(4,1)+SUM(5,1)*SUM(2,1))/(SUM(6,1)**2-
     XSUM(3,1)*SUM(2,1))
      B(3,1) = 0.
      C = CUE(1)-0.5*SUM(2,1)*B(1,1)**2-0.5*SUM(3,1)*B(2,1)**2+
     XSUM(4,1)*B(1,1)+SUM(5,1)*B(2,1)+SUM(6,1)*B(1,1)*B(2,1)
      PH=EXPF(C)
      DO 132 I=1,N
      CCUE(I)=SUM(1,1)-.5*SUM(2,1)*X(I)**2-.5*SUM(3,1)*Y(I)**2+SUM(4,1)
     X*X(I)+SUM(5,1)*Y(I)+SUM(6,1)*X(I)*Y(I)
      CCUE(I)=EXPF(CCUE(I))
  132 DELTA(I)=RHO(II,I)-CCUE(I)
      L = 3
      GO TO 50
   82 WRITE OUTPUT TAPE 6,114
      WRITE OUTPUT TAPE 6,110,(SUM(I,1),I=1,6)
      GO TO 90
      END  (   1 ,   1 ,   0 ,   1 ,   0   )
```

EXTERNAL FORMULA NUMBERS WITH CORRESPONDING INTERNAL FORMULA NUMBERS AND OCTAL LOCATIONS

EFN	IFN	LOC	EFN	IFN	LOC	EFN	IFN	LOC	EFN	IFN	LOC	EFN	IFN	LOC
100	2	00000	102	3	00000	104	4	00000	105	5	00000	106	6	00000
108	7	00000	999	8	00000	109	9	00000	110	10	00000	111	11	00000
112	12	00000	113	13	00000	114	14	00000	115	15	00000	116	16	00000
117	17	00000	118	18	00000	119	19	00000	121	20	00000	122	21	00000
126	22	00000	1	23	00012	1	24	00021	127	25	00023	127	27	00041
128	57	00212	128	63	00235	2	66	00257	4	68	00264	5	71	00300
6	73	00305	7	76	00321	8	78	00326	3	81	00341	9	82	00342
10	98	00476	11	101	00511	15	128	00606	16	139	00637	129	151	01110
50	152	01116	83	156	01135	90	173	01217	90	174	01226	91	178	01251
39	212	01447	20	213	01454	21	215	01455	22	233	01541	69	235	01545
23	237	01554	26	244	01626	130	255	02050	80	258	02063	80	259	02072
24	267	02115	33	274	02167	131	285	02411	81	288	02424	81	289	02433
25	297	02456	35	304	02530	132	315	02752	82	318	02765	82	319	02774

STORAGE NOT USED BY PROGRAM

DEC	OCT	DEC	OCT
2749	05275	32562	77462

LOCATIONS OF NAMES IN TRANSFER VECTOR

	DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT
EXP	0	00000	LOG	2	00002	MATINV	1	00001	(FIL)	3	00003	(IOH)I	8	00010
(IOH)O	5	00005	(LEV)	9	00011	(RTN)	6	00006	(STH)	4	00004	(TSH)	7	00007

STORAGE LOCATIONS FOR VARIABLES APPEARING IN DIMENSION AND EQUIVALENCE SENTENCES

	DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT
DELTA	2610	05062	CUE	2664	05150	CCUE	2637	05115	B	1774	03356	A	2174	04176
AA	2583	05027	KX	2572	05014	KY	2545	04761	KZ	2518	04726	REAL	2667	05153
RHO	2471	04647	R	1754	03332	SUM	2491	04673	X	2748	05274	Y	2721	05241
Z	2694	05206												

STORAGE LOCATIONS FOR VARIABLES NOT APPEARING IN DIMENSION,EQUIVALENCE OR COMMON SENTENCES

	DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT
II	1724	03274	C	1723	03273	ANY	1722	03272	K	1721	03271	L	1720	03270
M	1719	03267	N	1718	03266	PH	1717	03265	SFX	1716	03264	SFY	1715	03263
SFZ	1714	03262	TOT1	1713	03261	TOT2	1712	03260	TOT3	1711	03257			

STORAGE LOCCATIONS FOR SYMBOLS NOT APPEARING IN SOURCE PROGRAM

	DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT		DEC	OCT
C)106	1710	03256	C)G5	1709	03255	C)G4	1708	03254	C)G2	1707	03253	8)V7	1651	03163
8)3U	1578	03052	8)3Q	1579	03053	8)3P	1581	03055	8)3N	1583	03057	8)3M	1594	03072
8)3L	1598	03076	8)3K	1601	03101	8)3J	1614	03116	8)3I	1622	03126	8)3H	1630	03136
8)3G	1638	03146	8)3F	1640	03150	8)3E	1642	03152	8)3D	1649	03161	8)3C	1658	03172
8)3A	1661	03175	8)39	1663	03177	8)38	1671	03207	8)36	1684	03224	8)34	1693	03235
1)	1695	03237	2)	1551	03017	3)	1560	03030	6)	1572	03044	7)	1694	03236

SUBROUTINES NOT PUNCHED FROM LIBRARY

(LEV) (IOH)I (TSH) (RTN) (IOH)O (STH) (FIL) LOG MATINV EXP

```
000000 EXP      BCD  1EXP
000001 MATINV   BCD  1MATINV
000002 LOG      BCD  1LOG
000003 (FIL)    BCD  1(FIL)
000004 (STH)    BCD  1(STH)
000005 (IOH)O   BCD  1(IOH)O
000006 (RTN)    BCD  1(RTN)
000007 (TSH)    BCD  1(TSH)
000010 (IOH)I   BCD  1(IOH)I
000011 (LEV)    BCD  1(LEV)
000012 23A      CAL  *
000013          XIT  (LEV)
000014          ETM
000015          CAL  (IOH)I
000016          SLW  1
000017          CAL  (TSH)
000020 25D1     NTR  8)3J,0,7
000021 24A      CAL  *
000022          XIT  (RTN)
000023 25A      CAL  *
000024          XIT  (LEV)
000025          ETM
000026          CAL  (IOH)I
000027          SLW  1
000030          CAL  (TSH)
000031 25D1     NTR  8)3U,0,7
000032 26A      ETM
000033          NTR  SFX
000034          NTR  SFY
000035          NTR  SF7
000036          NTR  K
000037          NTR  N
000040          LTM
000041 27A      CAL  *
000042          XIT  (RTN)
000043 28A      CAL  *
000044          XIT  (LEV)
000045          ETM
000046          CAL  (IOH)I
000047          SLW  1
000050          CAL  (TSH)
000051 28D1     NTR  8)39,0,7
000052 29A      LXD  2)+2,2
000053          CLA  K
000054          STD  30A2
000055 30A      ETM
000056          NTR  R+1,2
000057          LTM
000060 30A1     TXI  *+1,2,1
000061 30A2     TXL  30A,2
000062 32A      LTM
000063 33A      CAL  *
000064          XIT  (RTN)
000065 34A      CAL  *
000066          XIT  (LEV)
000067          ETM
000070          CAL  (IOH)I
000071          SLW  1
000072          CAL  (TSH)
000073 34D1     NTR  8)39,0,7
000074 35A      LXD  2)+2,2
000075          CLA  K
000076          STD  36A2
000077 36A      ETM
000100          NTR  R-9,2
000101          LTM
000102 36A1     TXI  *+1,2,1
000103 36A2     TXL  36A,2
000104 38A      LTM
000105 39A      CAL  *
000106          XIT  (RTN)
000107 40A      CAL  *
000110          XIT  (LEV)
000111          ETM
000112          CAL  (IOH)I
000113          SLW  1
000114          CAL  (TSH)
000115 40D1     NTR  8)39,0,7
000116 41A      LXD  2)+2,2
000117          CLA  K
000120          STD  42A2
000121 42A      ETM
000122          NTR  R-19,2
000123          LTM
000124 42A1     TXI  *+1,2,1
000125 42A2     TXL  42A,2
000126 44A      LTM
000127 45A      CAL  *
000130          XIT  (RTN)
000131 46A      CAL  *
000132          XIT  (LEV)
000133          ETM
000134          CAL  (IOH)I
000135          SLW  1
000136          CAL  (TSH)
000137 46D1     NTR  8)3N,0,7
000140 47A      LXD  2)+2,2
000141          CLA  K
000142          STD  48A2
000143 48A      ETM
000144          NTR  AA+1,2
000145          LTM
000146 48A1     TXI  *+1,2,1
000147 48A2     TXL  48A,2
000150 50A      LTM
000151 51A      CAL  *
000152          XIT  (RTN)
000153 52A      CAL  *
000154          XIT  (LEV)
000155          ETM
000156          CAL  (IOH)O
000157          SLW  1
000160          CAL  (STH)
000161 52D1     NTR  8)34,0,6
000162 53A      CAL  *
000163          XIT  (FIL)
000164 54A      CAL  *
000165          XIT  (LEV)
000166          ETM
000167          CAL  (IOH)O
000170          SLW  1
000171          CAL  (STH)
000172 54D1     NTR  8)3J,0,6
000173 55A      CAL  *
000174          XIT  (FIL)
000175 56A      LXD  2)+2,2
000176          CLA  K
000177          STD  60A2
000200          CLA  K
000201          SUB  6)+3
000202          STD  63A3
000203          ADD  2)+8
000204          STD  63A1
000205          CLA  K
000206          STD  60A3
000207          LXD  2)+2,4
000210          CLA  N
000211          STD  63A4
000212 57A      CAL  *
000213          XIT  (LEV)
000214          ETM
000215          CAL  (IOH)I
000216          SLW  1
000217          CAL  (TSH)
000220 57D1     NTR  8)3A,0,7
000221 58A      ETM
000222          NTR  X+ ,4
000223          NTR  Y+ ,4
000224          NTR  Z+ ,4
000225          LTM
        59A     BSS
000226 60A      ETM
000227          NTR  RH0+1,2
000230          LTM
000231 60A1     TXI  *+1,2,1
000232 60A2     TXL  60A,2
000233 60A3     TIX  60A3+1,2
000234 62A      LTM
000235 63A      CAL  *
000236          XIT  (RTN)
000237 63A1     TXI  63A1+1,2
000240          SXD  60A2,2
000241 63A3     TIX  63A3+1,2
000242          TXI  *+ ,4,1
000243 63A4     TXL  57A,4
000244 64A      CLA  2)
000245          STO  II
000246          LXD  II,2
000247          SXD  C)G2,2
000250          LXD  II,4
000251          SXD  C)106,4
000252 65A      CLA  N
000253          SUB  2)+1
000254 65A1     TZE  66A
000255          TPL  81A
000256          TRA  81A
000257 66A      CLA  3)
000260          STO  TOT1
000261 67A      LXD  2)+2,4
000262          CLA  N
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00263          STD  68A2
00264  68A     CLA  X+1,4
00265          SSP
00266          FAD  TOT1
00267          STO  TOT1
00270  68A1    TXI  *+1,4,1
00271  68A2    TXL  68A,4
00272  69A     CLA  2)+2
00273          STO  M
00274          LXD  M,4
00275          SXD  C)G5,4
00276  70A     CLA  TOT1
00277  70A1    TZE  213A
00300  71A     CLA  3)
00301          STO  TOT2
00302  72A     LXD  2)+2,4
00303          CLA  N
00304          STD  72A2
00305  73A     CLA  Y+1,4
00306          SSP
00307          FAD  TOT2
00310          STO  TOT2
00311  73A1    TXI  *+1,4,1
00312  73A2    TXL  73A,4
00313  74A     CLA  2)+3
00314          STO  M
00315          LXD  M,4
00316          SXD  C)G5,4
00317  75A     CLA  TOT2
00320  75A1    TZE  213A
00321  76A     CLA  3)
00322          STO  TOT3
00323  77A     LXD  2)+2,4
00324          CLA  N
00325          STD  78A2
00326  78A     CLA  Z+1,4
00327          SSP
00330          FAD  TOT3
00331          STO  TOT3
00332  78A1    TXI  *+1,4,1
00333  78A2    TXL  78A,4
00334  79A     CLA  2)+4
00335          STO  M
00336          LXD  M,4
00337          SXD  C)G5,4
00340  80A     TRA  213A
00341  81A     LXD  2)+2,2
00342  82A     STZ  SUM+1,2
00343  82A1    TXI  *+1,2,1
00344  82A2    TXL  82A,2,20
00345  83A     CLA  II
00346          ADD  2)+2
00347          STO  II
00350          LXD  II,2
00351          SXD  C)G2,2
00352          LXD  II,4
00353          SXD  C)106,4
00354  84A     CAL  *
00355          XIT  (LEV)
00356          ETM

00357          CAL  (ICH)0
00360          SLW  1
00361          CAL  (STH)
00362  84D1    NTR  8)3P,0,6
00363  85A     ETM
00364          NTR  AA+1,2
00365          LTM
00366  86A     CAL  *
00367          XIT  (FIL)
00370  87A     LXD  2)+2,1
00371          CLA  N
00372          STD  98A2
00373          LXD  II,2
00374  88A     CLA  RHO+1,2
00375          SXD  6)+4,4
00376          TSX  LOG,4
00377          NTR  *+2,0,9
00400          PZE  0,0,88
00401          LXD  6)+4,4
00402          STO  CUE+1,1
00403  89A     CLA  SUM
00404          FAD  CUE+1,1
00405          STO  SUM
00406  90A     LDQ  X+1,1
00407          FMP  X+1,1
00410          STO  1)+1
00411          LDQ  CUE+1,1
00412          FMP  3)+1
00413          STO  7)
00414          LDQ  7)
00415          FMP  1)+1
00416          FAD  SUM-1
00417          STO  SUM-1
00420  91A     LDQ  Y+1,1
00421          FMP  Y+1,1
00422          STO  1)+1
00423          LDQ  CUE+1,1
00424          FMP  3)+1
00425          STO  7)
00426          LDQ  7)
00427          FMP  1)+1
00430          FAD  SUM-2
00431          STO  SUM-2
00432  92A     LDQ  Z+1,1
00433          FMP  Z+1,1
00434          STO  1)+1
00435          LDQ  CUE+1,1
00436          FMP  3)+1
00437          STO  7)
00440          LDQ  7)
00441          FMP  1)+1
00442          FAD  SUM-3
00443          STO  SUM-3
00444  93A     LDQ  X+1,1
00445          FMP  CUE+1,1
00446          FAD  SUM-4
00447          STO  SUM-4
00450  94A     LDQ  Y+1,1
00451          FMP  CUE+1,1
00452          FAD  SUM-5

00453          STO  SUM-5
00454  95A     LDQ  Z+1,1
00455          FMP  CUE+1,1
00456          FAD  SUM-6
00457          STO  SUM-6
00460  96A     LDQ  CUE+1,1
00461          FMP  Y+1,1
00462          STO  7)
00463          LDQ  7)
00464          FMP  Z+1,1
00465          FAD  SUM-7
00466          STO  SUM-7
00467  97A     LDQ  CUE+1,1
00470          FMP  X+1,1
00471          STO  7)
00472          LDQ  7)
00473          FMP  Z+1,1
00474          FAD  SUM-8
00475          STO  SUM-8
00476  98A     LDQ  CUE+1,1
00477          FMP  X+1,1
00500          STO  7)
00501          LDQ  7)
00502          FMP  Y+1,1
00503          FAD  SUM-9
00504          STO  SUM-9
00505  98A1    TXI  *+1,1,1
00506          TXI  *+1,2,11
00507  98A2    TXL  88A,1
00510  99A     LXD  2)+2,1
               100A BSS
00511  100A    STZ  A+1,1
00512  100A1   TXI  *+1,1,20
00513  100A2   TXL  10 A,1,400
00514  100A3   TIX  10 A+1,1,400
00515  100A4   TXI  *+1,1,1
00516  100A5   TXL  10 A,1,20
00517  102A    CLA  3)+2
00520          STO  A
00521  103A    CLA  3)+3
00522          STO  A-
00523  104A    CLA  3)+3
00524          STO  A-
00525  105A    CLA  3)+3
00526          STO  A-
00527  106A    CLS  3)+3
00530          STO  A- 0
00531  107A    CLS  3)+4
00532          STO  A- 1
00533  108A    CLS  3)+5
00534          STO  A- 2
00535  109A    CLS  3)+5
00536          STO  A-3
00537  110A    CLS  3)+3
00540          STO  A- 0
00541  111A    CLS  3)+5
00542          STO  A- 1
00543  112A    CLS  3)+4
00544          STO  A- 2
00545  113A    CLS  3)+5
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00546          STO  A-43
00547  114A    CLS  3)+3
00550          STO  A-60
00551  115A    CLS  3)+5
00552          STO  A-61
00553  116A    CLS  3)+5
00554          STO  A-62
00555  117A    CLS  3)+4
00556          STO  A-63
00557  118A    CLA  3)+6
00560          STO  A-84
00561  119A    CLA  3)+6
00562          STO  A-105
00563  120A    CLA  3)+6
00564          STO  A-126
00565  121A    CLA  3)+7
00566          STO  A-147
00567  122A    CLA  3)+7
00570          STO  A-168
00571  123A    CLA  3)+7
00572          STO  A-189
00573  124A    SXD  6)+4,4
00574  125A    TSX  MATINV,4
00575          PZE  A
00576          PZE  2)+5
00577          PZE  SUM
00600          PZE  2)+2
00601          PZE  ANY
00602          NTR  *+2,0,11
00603          PZE  0,0,125
00604          LXD  6)+4,4
00605  126A    LXD  2)+2,1
       127A    BSS
00606  128A    STZ  A+1,1
00607  128A1   TXI  *+1,1,20
00610  128A2   TXL  128A,1,400
00611  128A3   TIX  128A3+1,1,400
00612  128A4   TXI  *+1,1,1
00613  128A5   TXL  127A,1,20
00614  129A    CLA  SUM-1
00615          STO  A
00616  130A    CLA  SUM-9
00617          STO  A-1
00620  131A    CLA  SUM-8
00621          STO  A-2
00622  132A    CLS  SUM-9
00623          STO  A-20
00624  133A    CLS  SUM-2
00625          STO  A-21
00626  134A    CLA  SUM-7
00627          STO  A-22
00630  135A    CLS  SUM-8
00631          STO  A-40
00632  136A    CLA  SUM-7
00633          STO  A-41
00634  137A    CLS  SUM-3
00635          STO  A-42
00636  138A    LXD  2)+2,1
00637  139A    STZ  B+1,1
00640  139A1   TXI  *+1,1,1
00641  139A2   TXL  139A,1,20
00642  140A    CLA  SUM-4
00643          STO  B
00644  141A    CLS  SUM-5
00645          STO  B-1
00646  142A    CLS  SUM-6
00647          STO  B-2
00650  143A    SXD  6)+4,4
00651  144A    TSX  MATINV,4
00652          PZE  A
00653          PZE  2)+4
00654          PZE  B
00655          PZE  2)+2
00656          PZE  ANY
00657          NTR  *+2,0,16
00660          PZE  0,0,144
00661          LXD  6)+4,4
00662  145A    CLA  2)+6
00663          STO  L
00664          LXD  L,1
00665          SXD  C)G4,1
00666  146A    LDQ  B-1
00667          FMP  SUM-9
00670          STO  7)
00671          LDQ  7)
00672          FMP  B
00673          STO  1)+1
00674          LDQ  B-2
00675          FMP  SUM-8
00676          STO  7)
00677          LDQ  7)
00700          FMP  B
00701          STO  1)+2
00702          LDQ  B-2
00703          FMP  SUM-7
00704          STO  7)
00705          LDQ  7)
00706          FMP  B-1
00707          STO  1)+3
00710          LDQ  SUM-6
00711          FMP  B-2
00712          STO  1)+4
00713          LDQ  SUM-5
00714          FMP  B-1
00715          STO  1)+5
00716          LDQ  SUM-4
00717          FMP  B
00720          STO  1)+6
00721          LDQ  B-2
00722          FMP  B-2
00723          STO  1)+7
00724          LDQ  1)+7
00725          FMP  3)+1
00726          STO  7)
00727          LDQ  7)
00730          FMP  SUM-3
00731          STO  1)+8
00732          LDQ  B-1
00733          FMP  B-1
00734          STO  1)+9
00735          LDQ  1)+9
00736          FMP  3)+1
00737          STO  7)
00740          LDQ  7)
00741          FMP  SUM-2
00742          STO  1)+10
00743          LDQ  B
00744          FMP  B
00745          STO  1)+11
00746          LDQ  1)+11
00747          FMP  3)+1
00750          STO  7)
00751          LDQ  7)
00752          FMP  SUM-1
00753          CHS
00754          FAD  CUF
00755          FSB  1)+10
00756          FSB  1)+8
00757          FAD  1)+6
00760          FAD  1)+5
00761          FAD  1)+4
00762          FAD  1)+3
00763          FAD  1)+2
00764          FAD  1)+1
00765          STO  C
00766  147A    CLA  C
00767          SXD  6)+4,4
00770          TSX  EXP,4
00771          NTR  *+2,0,16
00772          PZE  0,0,147
00773          LXD  6)+4,4
00774          STO  PH
00775  148A    LXD  2)+2,2
00776          CLA  N
00777          STD  15A2
01000          LXD  11,1
01001  149A    LDQ  X+1,2
01002          FMP  SUM-9
01003          STO  7)
01004          LDQ  7)
01005          FMP  Y+1,2
01006          STO  1)+1
01007          LDQ  Z+1,2
01010          FMP  SUM-8
01011          STO  7)
01012          LDQ  7)
01013          FMP  X+1,2
01014          STO  1)+2
01015          LDQ  Z+1,2
01016          FMP  SUM-7
01017          STO  7)
01020          LDQ  7)
01021          FMP  Y+1,2
01022          STO  1)+3
01023          LDQ  SUM-6
01024          FMP  Z+1,2
01025          STO  1)+4
01026          LDQ  SUM-5
01027          FMP  Y+1,2
01030          STO  1)+5
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01031          LDQ  SUM-4
01032          FMP  X+1,2
01033          STO  1)+6
01034          LDQ  Z+1,2
01035          FMP  Z+1,2
01036          STO  1)+7
01037          LDQ  1)+7
01040          FMP  3)+1
01041          STO  7)
01042          LDQ  7)
01043          FMP  SUM-3
01044          STO  1)+8
01045          LDQ  Y+1,2
01046          FMP  Y+1,2
01047          STO  1)+9
01050          LDQ  1)+9
01051          FMP  3)+1
01052          STO  7)
01053          LDQ  7)
01054          FMP  SUM-2
01055          STO  1)+10
01056          LDQ  X+1,2
01057          FMP  X+1,2
01060          STO  1)+11
01061          LDQ  1)+11
01062          FMP  3)+1
01063          STO  7)
01064          LDQ  7)
01065          FMP  SUM-1
01066          CHS
01067          FAD  SUM
01070          FSB  1)+10
01071          FSB  1)+8
01072          FAD  1)+6
01073          FAD  1)+5
01074          FAD  1)+4
01075          FAD  1)+3
01076          FAD  1)+2
01077          FAD  1)+1
01100          STO  CCUE+1,2
01101  150A    CLA  CCUE+1,2
01102          SXD  6)+4,4
01103          TSX  EXP,4
01104          NTR  *+2,C,16
01105          PZE  0,0,150
01106          LXD  6)+4,4
01107          STO  CCUE+1,2
01110  151A    CLA  RHO+1,1
01111          FSB  CCUE+1,2
01112          STO  DELTA+1,2
01113  151A1   TXI  *+1,2,1
01114          TXI  *+1,1,11
01115  151A2   TXL  149A,2
01116  152A    CLA  B
01117          FAD  R+1,4
01120          STO  REAL
01121  153A    CLA  B-1
01122          FAD  R-9,4
01123          STO  REAL-1
01124  154A    CLA  B-2
01125          FAD  R-19,4
01126          STO  REAL-2
01127          LXD  C)G4,1
01130  155A    TRA  155A+5,1
01131          TRA  156A
01132          TRA  318A
01133          TRA  288A
01134          TRA  258A
       156A    BSS
01135  157A    CAL  *
01136          XIT  (LEV)
01137          ETM
01140          CAL  (IOH)O
01141          SLW  1
01142          CAL  (STH)
01143  157D1   NTR  8)3C,0,6
01144  158A    CAL  *
01145          XIT  (FIL)
01146  159A    CAL  *
01147          XIT  (LEV)
01150          ETM
01151          CAL  (IOH)O
01152          SLW  1
01153          CAL  (STH)
01154  159D1   NTR  8)3E,0,6
01155  160A    LXD  2)+2,2
01156  161A    ETM
01157          NTR  SUM+1,2
01160          LTM
01161  161A1   TXI  *+1,2,1
01162  161A2   TXL  161A,2,5
01163  163A    LTM
01164  164A    CAL  *
01165          XIT  (FIL)
01166  165A    CAL  *
01167          XIT  (LEV)
01170          ETM
01171          CAL  (IOH)O
01172          SLW  1
01173          CAL  (STH)
01174  165D1   NTR  8)3D,0,6
01175  166A    CAL  *
01176          XIT  (FIL)
01177  167A    CAL  *
01200          XIT  (LEV)
01201          ETM
01202          CAL  (IOH)O
01203          SLW  1
01204          CAL  (STH)
01205  167D1   NTR  8)3E,0,6
01206  168A    LXD  2)+7,2
01207  169A    ETM
01210          NTR  SUM+1,2
01211          LTM
01212  169A1   TXI  *+1,2,1
01213  169A2   TXL  169A,2,10
01214  171A    LTM
01215  172A    CAL  *
01216          XIT  (FIL)
01217  173A    CAL  *
01220          XIT  (LEV)
01221          ETM
01222          CAL  (IOH)O
01223          SLW  1
01224          CAL  (STH)
01225  173D1   NTR  8)36,0,6
01226  174A    CAL  *
01227          XIT  (FIL)
01230  175A    LXD  2)+2,2
01231          CLA  N
01232          STD  178A2
01233  176A    CLA  X+1,2
01234          UFA  6)
01235          LRS
01236          ANA  6)+1
01237          LLS
01240          ALS  18
01241          STO  KX+1,2
01242  177A    CLA  Y+1,2
01243          UFA  6)
01244          LRS
01245          ANA  6)+1
01246          LLS
01247          ALS  18
01250          STO  KY+1,2
01251  178A    CLA  Z+1,2
01252          UFA  6)
01253          LRS
01254          ANA  6)+1
01255          LLS
01256          ALS  18
01257          STO  KZ+1,2
01260  178A1   TXI  *+1,2,1
01261  178A2   TXL  176A,2
01262  179A    CAL  *
01263          XIT  (LEV)
01264          ETM
01265          CAL  (IOH)O
01266          SLW  1
01267          CAL  (STH)
01270  179D1   NTR  8)3L,0,6
01271  180A    LXD  2)+2,2
01272          CLA  N
01273          STD  181A2
01274          LXD  11,4
01275  181A    ETM
01276          NTR  KX+1,2
01277          NTR  KY+1,2
01300          NTR  KZ+1,2
01301          NTR  RHO+1,4
01302          NTR  CCUE+1,2
01303          NTR  DELTA+1,2
01304          LTM
01305  181A1   TXI  *+1,2,1
01306          TXI  *+1,4,11
01307  181A2   TXL  181A,2
01310  183A    LTM
01311  184A    CAL  *
01312          XIT  (FIL)
01313  185A    CAL  *
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013 4          XIT  (LEV)
01315          ETM
01316          CAL  (ICH)0
01317          SLW  1
01320          CAL  (STH)
01321 185D1    NTR  8)38,0,6
01322 186A     CAL  *
01323          XIT  (FIL)
01324 187A     CAL  *
01325          XIT  (LEV)
01326          ETM
01327          CAL  (IOH)0
01330          SLW  1
01331          CAL  (STH)
01332 187D1    NTR  8)3F,0,6
01333 188A     LXD  2)+2,2
01334 189A     ETM
01335          NTR  REAL+1,2
01336          LTM
01337 189A1    TXI  *+1,2,1
01340 189A2    TXL  189A,2,3
01341 191A     LTM
01342 192A     CAL  *
01343          XIT  (FIL)
01344 193A     LDQ  REAL
01345          FMP  SFX
01346          STO  REAL
01347 194A     LDQ  REAL-1
01350          FMP  SFY
01351          STO  REAL-1
01352 195A     LDQ  REAL-2
01353          FMP  SFZ
01354          STO  REAL-2
01355 196A     CAL  *
01356          XIT  (LEV)
01357          ETM
01360          CAL  (IOH)0
01361          SLW  1
01362          CAL  (STH)
01363 196D1    NTR  8)3M,0,6
01364 197A     CAL  *
01365          XIT  (FIL)
01366 198A     CAL  *
01367          XIT  (LEV)
01370          ETM
01371          CAL  (IOH)0
01372          SLW  1
01373          CAL  (STH)
01374 198D1    NTR  8)3F,0,6
01375 199A     LXD  2)+2,2
01376 200A     ETM
01377          NTR  REAL+1,2
01400          LTM
01401 200A1    TXI  *+1,2,1
01402 200A2    TXL  200A,2,3
01403 202A     LTM
01404 203A     CAL  *
01405          XIT  (FIL)
01406 204A     CAL  *
01407          XIT  (LEV)

01410          ETM
01411          CAL  (IOH)0
01412          SLW  1
01413          CAL  (STH)
01414 204D1    NTR  8)3K,0,6
01415 205A     CAL  *
01416          XIT  (FIL)
01417 206A     CAL  *
01420          XIT  (LEV)
01421          ETM
01422          CAL  (IOH)0
01423          SLW  1
01424          CAL  (STH)
01425 206D1    NTR  8)V7,0,6
01426 207A     ETM
01427          NTR  PH
01430          LTM
01431 208A     CAL  *
01432          XIT  (FIL)
01433 209A     CAL  *
01434          XIT  (LEV)
01435          ETM
01436          CAL  (IOH)0
01437          SLW  1
01440          CAL  (STH)
01441 209D1    NTR  8)3Q,0,6
01442 210A     CAL  *
01443          XIT  (FIL)
01444 211A     CLA  II
01445          SUB  K
01446 211A1    TZE  23A
01447 212A     CLA  N
01450          SUB  2)+1
01451 212A1    TZE  213A
01452          TPL  81A
01453          TRA  81A
01454 213A     LXD  2)+2,2
              214A  BSS
01455 215A     STZ  A+1,2
01456 215A1    TXI  *+1,2,20
01457 215A2    TXL  215A,2,400
01460 215A3    TIX  215A3+1,2,400
01461 215A4    TXI  *+1,2,1
01462 215A5    TXL  214A,2,20
01463 216A     CLA  3)+3
01464          STO  A
01465 217A     CLA  3)+5
01466          STO  A-1
01467 218A     CLA  3)+5
01470          STO  A-2
01471 219A     CLS  3)+5
01472          STO  A-21
01473 220A     CLS  3)+8
01474          STO  A-21
01475 221A     CLS  3)+9
01476          STO  A-22
01477 222A     CLS  3)+5
01500          STO  A-40
01501 223A     CLS  3)+9
01502          STO  A-41

01503 224A     CLS  3)+8
01504          STO  A-42
01505 225A     CLA  3)+10
01506          STO  A-63
01507 226A     CLA  3)+10
01510          STO  A-84
01511 227A     CLA  3)+11
01512          STO  A-105
01513 228A     CLA  II
01514          ADD  2)+2
01515          STO  II
01516          LXD  II,2
01517          SXD  C)G2,2
01520          LXD  II,4
01521          SXD  C)106,4
01522 229A     CAL  *
01523          XIT  (LEV)
01524          ETM
01525          CAL  (IOH)0
01526          SLW  1
01527          CAL  (STH)
01530 229D1    NTR  8)3P,0,6
01531 230A     ETM
01532          NTR  AA+1,2
01533          LTM
01534 231A     CAL  *
01535          XIT  (FIL)
01536 232A     LXD  2)+2,1
01537          CLA  N
01540          STD  232A2
01541 233A     STZ  SUM+1,1
01542 233A1    TXI  *+1,1,1
01543 233A2    TXL  232A,1
01544 234A     LXD  2)+2,1
01545 235A     STZ  B+1,1
01546 235A1    TXI  *+1,1,1
01547 235A2    TXL  235A,1,20
01550          LXD  C)G5,1
01551 236A     TRA  236A+4,1
01552          TRA  297A
01553          TRA  267A
01554 237A     LXD  2)+2,2
01555          CLA  N
01556          STD  244A2
01557          LXD  II,1
01560 238A     CLA  RHO+1,1
01561          SXD  6)+4,4
01562          TSX  LOG,4
01563          NTR  *+2,0,23
01564          PZE  0,1,238
01565          LXD  6)+4,4
01566          STO  CUE+1,2
01567 239A     CLA  SUM
01570          FAD  CUE+1,2
01571          STO  SUM
01572 240A     LDQ  Y+1,2
01573          FMP  Y+1,2
01574          STO  1)+1
01575          LDQ  CUE+1,2
01576          FMP  3)+1
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01577           STO  7)
01600           LDQ  7)
01601           FMP  1)+1
01602           FAD  SUM-1
01603           STO  SUM-1
01604  241A    LDQ  Z+1,2
01605           FMP  Z+1,2
01606           STO  1)+1
01607           LDQ  CUE+1,2
01610           FMP  3)+1
01611           STO  7)
01612           LDQ  7)
01613           FMP  1)+1
01614           FAD  SUM-2
01615           STO  SUM-2
01616  242A    LDQ  Y+1,2
01617           FMP  CUE+1,2
01620           FAD  SUM-3
01621           STO  SUM-3
01622  243A    LDQ  Z+1,2
01623           FMP  CUE+1,2
01624           FAD  SUM-4
01625           STO  SUM-4
01626  244A    LDQ  CUE+1,2
01627           FMP  Y+1,2
01630           STO  7)
01631           LDQ  7)
01632           FMP  Z+1,2
01633           FAD  SUM-5
01634           STO  SUM-5
01635  244A1   TXI  *+1,2,1
01636           TXI  *+1,1,11
01637  244A2   TXL  238A,2
01640  245A    SXD  6)+4,4
01641  246A    TSX  MATINV,4
01642           PZE  A
01643           PZE  2)+7
01644           PZE  SUM
01645           PZE  2)+2
01646           PZE  ANY
01647           NTR  *+2,0,26
01650           PZE  0,0,246
01651           LXD  6)+4,4
01652  247A    CLA  3)
01653           STO  B
01654  248A    LDQ  SUM-1
01655           FMP  SUM-2
01656           STO  1)+1
01657           LDQ  SUM-5
01660           FMP  SUM-5
01661           FSB  1)+1
01662           STO  1)+2
01663           LDQ  SUM-5
01664           FMP  SUM-4
01665           STO  1)+3
01666           LDQ  SUM-3
01667           FMP  SUM-2
01670           FAD  1)+3
01671           FDP  1)+2
01672           STQ  1)+4
01673           CLS  1)+4
01674           STO  B-1
01675  249A    LDQ  SUM-1
01676           FMP  SUM-2
01677           STO  1)+1
01700           LDQ  SUM-5
01701           FMP  SUM-5
01702           FSB  1)+1
01703           STO  1)+2
01704           LDQ  SUM-3
01705           FMP  SUM-5
01706           STO  1)+3
01707           LDQ  SUM-1
01710           FMP  SUM-4
01711           FAD  1)+3
01712           FDP  1)+2
01713           STQ  1)+4
01714           CLS  1)+4
01715           STO  B-2
01716  250A    LDQ  B-2
01717           FMP  SUM-5
01720           STO  7)
01721           LDQ  7)
01722           FMP  B-1
01723           STO  1)+1
01724           LDQ  SUM-4
01725           FMP  B-2
01726           STO  1)+2
01727           LDQ  SUM-3
01730           FMP  B-1
01731           STO  1)+3
01732           LDQ  B-2
01733           FMP  B-2
01734           STO  1)+4
01735           LDQ  1)+4
01736           FMP  3)+1
01737           STO  7)
01740           LDQ  7)
01741           FMP  SUM-2
01742           STO  1)+5
01743           LDQ  B-1
01744           FMP  B-1
01745           STO  1)+6
01746           LDQ  1)+6
01747           FMP  3)+1
01750           STO  7)
01751           LDQ  7)
01752           FMP  SUM-1
01753           CHS
01754           FAD  CUE
01755           FSB  1)+5
01756           FAD  1)+3
01757           FAD  1)+2
01760           FAD  1)+1
01761           STO  C
01762  251A    CLA  C
01763           SXD  6)+4,4
01764           TSX  EXP,4
01765           NTR  *+2,0,26
01766           PZE  0,0,251
01767           LXD  6)+4,4
01770           STO  PH
01771  252A    LXD  2)+2,1
01772           CLA  N
01773           STD  253A2
01774           LXD  11,2
01775  253A    LDQ  Z+ ,1
01776           FMP  SUM-5
01777           STO  7)
02000           LDQ  7)
02001           FMP  Y+ ,1
02002           STO  1)+1
02003           LDQ  SUM-4
02004           FMP  Z+ ,1
02005           STO  1)+2
02006           LDQ  SUM-3
02007           FMP  Y+ ,1
02010           STO  1)+3
02011           LDQ  Z+ ,1
02012           FMP  Z+ ,1
02013           STO  1)+4
02014           LDQ  1)+4
02015           FMP  3)+1
02016           STO  7)
02017           LDQ  7)
02020           FMP  SUM-2
02021           STO  1)+5
02022           LDQ  Y+ ,1
02023           FMP  Y+ ,1
02024           STO  1)+6
02025           LDQ  1)+6
02026           FMP  3)+1
02027           STO  7)
02030           LDQ  7)
02031           FMP  SUM-1
02032           CHS
02033           FAD  SUM
02034           FSB  1)+5
02035           FAD  1)+3
02036           FAD  1)+2
02037           FAD  1)+1
02040           STO  CCUE+1,1
02041  254A    CLA  CCUE+1,1
02042           SXD  6)+4,4
02043           TSX  EXP,4
02044           NTR  *+ ,0,26
02045           PZE  0,0,254
02046           LXD  6)+4,4
02047           STO  CCUE+1,1
02050  255A    CLA  RHO+1,2
02051           FSB  CCUE+1,1
02052           STO  DELTA+1,1
02053  255A1   TXI  *+ ,1,1
02054           TXI  *+ ,2,1
02055  255A2   TXL  253A,1
02056  256A    CLA  2)+2
02057           STO  L
02060           LXD  L,
02061           SXD  C)G4,1
02062  257A    TRA  150A
```

```
02063 258A    CAL  *
02064         XIT  (LEV)
02065         ETM
02066         CAL  (IOH)0
02067         SLW  1
02070         CAL  (STH)
02071 258D1   NTR  8)3G,0,6
02072 259A    CAL  *
02073         XIT  (FIL)
02074 260A    CAL  *
02075         XIT  (LEV)
02076         ETM
02077         CAL  (IOH)0
02100         SLW  1
02101         CAL  (STH)
02102 260D1   NTR  8)3E,0,6
02103 261A    LXD  2)+2,2
02104 262A    ETM
02105         NTR  SUM+1,2
02106         LTM
02107 262A1   TXI  *+1,2,1
02110 262A2   TXL  262A,2,6
02111 264A    LTM
02112 265A    CAL  *
02113         XIT  (FIL)
02114 266A    TRA  173A
02115 267A    LXD  2)+2,2
02116         CLA  N
02117         STD  274A2
02120         LXD  II,1
02121 268A    CLA  RHO+1,1
02122         SXD  6)+4,4
02123         TSX  LOG,4
02124         NTR  *+2,0,24
02125         PZE  0,0,268
02126         LXD  6)+4,4
02127         STO  CUE+1,2
02130 269A    CLA  SUM
02131         FAD  CUE+1,2
02132         STO  SUM
02133 270A    LDQ  X+1,2
02134         FMP  X+1,2
02135         STO  1)+1
02136         LDQ  CUE+1,2
02137         FMP  3)+1
02140         STO  7)
02141         LDQ  7)
02142         FMP  1)+1
02143         FAD  SUM-1
02144         STO  SUM-1
02145 271A    LDQ  Z+1,2
02146         FMP  Z+1,2
02147         STO  1)+1
02150         LDQ  CUE+1,2
02151         FMP  3)+1
02152         STO  7)
02153         LDQ  7)
02154         FMP  1)+1
02155         FAD  SUM-2
02156         STO  SUM-2

02157 272A    LDQ  X+1,2
02160         FMP  CUE+1,2
02161         FAD  SUM-3
02162         STO  SUM-3
02163 273A    LDQ  Z+1,2
02164         FMP  CUE+1,2
02165         FAD  SUM-4
02166         STO  SUM-4
02167 274A    LDQ  CUE+1,2
02170         FMP  X+1,2
02171         STO  7)
02172         LDQ  7)
02173         FMP  Z+1,2
02174         FAD  SUM-5
02175         STO  SUM-5
02176 274A1   TXI  *+1,2,1
02177         TXI  *+1,1,11
02200 274A2   TXL  268A,2
02201 275A    SXD  6)+4,4
02202 276A    TSX  MATINV,4
02203         PZE  A
02204         PZE  2)+7
02205         PZE  SUM
02206         PZE  2)+2
02207         PZE  ANY
02210         NTR  *+2,0,33
02211         PZE  0,0,276
02212         LXD  6)+4,4
02213 277A    LDQ  SUM-2
02214         FMP  SUM-1
02215         STO  1)+1
02216         LDQ  SUM-5
02217         FMP  SUM-5
02220         FSB  1)+1
02221         STO  1)+2
02222         LDQ  SUM-2
02223         FMP  SUM-3
02224         STO  1)+3
02225         LDQ  SUM-4
02226         FMP  SUM-5
02227         FAD  1)+3
02230         FDP  1)+2
02231         STQ  1)+4
02232         CLS  1)+4
02233         STO  B
02234 278A    CLA  3)
02235         STO  B-1
02236 279A    LDQ  SUM-2
02237         FMP  SUM-1
02240         STO  1)+1
02241         LDQ  SUM-5
02242         FMP  SUM-5
02243         FSB  1)+1
02244         STO  1)+2
02245         LDQ  SUM-5
02246         FMP  SUM-3
02247         STO  1)+3
02250         LDQ  SUM-4
02251         FMP  SUM-1
02252         FAD  1)+3

02253         FDP  1)+2
02254         STQ  1)+4
02255         CLS  1)+4
02256         STO  B-1
02257 280A    LDQ  B-1
02260         FMP  SUM-5
02261         STO  7)
02262         LDQ  7)
02263         FMP  B
02264         STO  1)+1
02265         LDQ  SUM-4
02266         FMP  B-1
02267         STO  1)+2
02270         LDQ  SUM-3
02271         FMP  B
02272         STO  1)+3
02273         LDQ  B-1
02274         FMP  B-2
02275         STO  1)+4
02276         LDQ  1)+4
02277         FMP  3)+1
02300         STO  7)
02301         LDQ  7)
02302         FMP  SUM-2
02303         STO  1)+5
02304         LDQ  B
02305         FMP  B
02306         STO  1)+6
02307         LDQ  1)+6
02310         FMP  3)+1
02311         STO  7)
02312         LDQ  7)
02313         FMP  SUM-1
02314         CHS
02315         FAD  CUE
02316         FSB  1)+5
02317         FAD  1)+3
02320         FAD  1)+2
02321         FAD  1)+1
02322         STO  C
02323 281A    CLA  C
02324         SXD  6)+4,4
02325         TSX  EXP,4
02326         NTR  *+2,0,33
02327         PZE  0,0,281
02330         LXD  6)+4,4
02331         STO  PH
02332 282A    LXD  2)+2,1
02333         CLA  N
02334         STD  285A2
02335         LXD  II,2
02336 283A    LDQ  Z+1,1
02337         FMP  SUM-5
02340         STO  7)
02341         LDQ  7)
02342         FMP  X+1,1
02343         STO  1)+1
02344         LDQ  SUM-4
02345         FMP  Z+1,1
02346         STO  1)+2
```

```
02347          LDQ  SUM-3
02350          FMP  X+1,1
02351          STO  1)+3
02352          LDQ  Z+1,1
02353          FMP  Z+1,1
02354          STO  1)+4
02355          LDQ  1)+4
02356          FMP  3)+1
02357          STO  7)
02360          LDQ  7)
02361          FMP  SUM-2
02362          STO  1)+5
02363          LDQ  X+1,1
02364          FMP  X+1,1
02365          STO  1)+6
02366          LDQ  1)+6
02367          FMP  3)+1
02370          STO  7)
02371          LDQ  7)
02372          FMP  SUM-1
02373          CHS
02374          FAD  SUM
02375          FSB  1)+5
02376          FAD  1)+3
02377          FAD  1)+2
02400          FAD  1)+1
02401          STO  CCUE+1,1
02402  284A   CLA  CCUE+1,1
02403          SXD  6)+4,4
02404          TSX  EXP,4
02405          NTR  *+2,0,33
02406          PZE  0,0,284
02407          LXD  6)+4,4
02410          STO  CCUE+1,1
02411  285A   CLA  RHO+1,2
02412          FSB  CCUE+1,1
02413          STO  DELTA+1,1
02414  285A1  TXI  *+1,1,1
02415          TXI  *+1,2,11
02416  285A2  TXL  283A,1
02417  286A   CLA  2)+3
02420          STO  L
02421          LXD  L,1
02422          SXD  C)G4,1
02423  287A   TRA  152A
02424  288A   CAL  *
02425          XIT  (LEV)
02426          ETM
02427          CAL  (IOH)O
02430          SLW  1
02431          CAL  (STH)
02432  288D1  NTR  8)3H,0,6
02433  289A   CAL  *
02434          XIT  (FIL)
02435  290A   CAL  *
02436          XIT  (LEV)
02437          ETM
02440          CAL  (IOH)O
02441          SLW  1
02442          CAL  (STH)

02443  290D1  NTR  8)3E,0,6
02444  291A   LXD  2)+2,2
02445  292A   ETM
02446          NTR  SUM+1,2
02447          LTM
02450  292A1  TXI  *+1,2,1
02451  292A2  TXL  292A,2,6
02452  294A   LTM
02453  295A   CAL  *
02454          XIT  (FIL)
02455  296A   TRA  173A
02456  297A   LXD  2)+2,2
02457          CLA  N
02460          STD  304A2
02461          LXD  II,1
02462  298A   CLA  RHO+1,1
02463          SXD  6)+4,4
02464          TSX  LOG,4
02465          NTR  *+2,0,25
02466          PZE  0,0,298
02467          LXD  6)+4,4
02470          STO  CUE+1,2
02471  299A   CLA  SUM
02472          FAD  CUE+1,2
02473          STO  SUM
02474  300A   LDQ  X+1,2
02475          FMP  X+1,2
02476          STO  1)+1
02477          LDQ  CUE+1,2
02500          FMP  3)+1
02501          STO  7)
02502          LDQ  7)
02503          FMP  1)+1
02504          FAD  SUM-1
02505          STO  SUM-1
02506  301A   LDQ  Y+1,2
02507          FMP  Y+1,2
02510          STO  1)+1
02511          LDQ  CUE+1,2
02512          FMP  3)+1
02513          STO  7)
02514          LDQ  7)
02515          FMP  1)+1
02516          FAD  SUM-2
02517          STO  SUM-2
02520  302A   LDQ  X+1,2
02521          FMP  CUE+1,2
02522          FAD  SUM-3
02523          STO  SUM-3
02524  303A   LDQ  Y+1,2
02525          FMP  CUE+1,2
02526          FAD  SUM-4
02527          STO  SUM-4
02530  304A   LDQ  CUE+1,2
02531          FMP  X+1,2
02532          STO  7)
02533          LDQ  7)
02534          FMP  Y+1,2
02535          FAD  SUM-5
02536          STO  SUM-5

02537  304A1  TXI  *+1,2,1
02540          TXI  *+1,1,11
02541  304A2  TXL  298A,2
02542  305A   SXD  6)+4,4
02543  306A   TSX  MATINV,4
02544          PZE  A
02545          PZE  2)+7
02546          PZE  SUM
02547          PZE  2)+2
02550          PZE  ANY
02551          NTR  *+2,0,35
02552          PZE  0,0,306
02553          LXD  6)+4,4
02554  307A   LDQ  SUM-2
02555          FMP  SUM-1
02556          STO  1)+1
02557          LDQ  SUM-5
02560          FMP  SUM-5
02561          FSB  1)+1
02562          STO  1)+2
02563          LDQ  SUM-5
02564          FMP  SUM-4
02565          STO  1)+3
02566          LDQ  SUM-3
02567          FMP  SUM-2
02570          FAD  1)+3
02571          FDP  1)+2
02572          STQ  1)+4
02573          CLS  1)+4
02574          STO  B
02575  308A   LDQ  SUM-2
02576          FMP  SUM-1
02577          STO  1)+1
02600          LDQ  SUM-5
02601          FMP  SUM-5
02602          FSB  1)+1
02603          STO  1)+2
02604          LDQ  SUM-4
02605          FMP  SUM-1
02606          STO  1)+3
02607          LDQ  SUM-5
02610          FMP  SUM-3
02611          FAD  1)+3
02612          FDP  1)+2
02613          STQ  1)+4
02614          CLS  1)+4
02615          STO  B-1
02616  309A   CLA  3)
02617          STO  B-2
02620  310A   LDQ  B-1
02621          FMP  SUM-5
02622          STO  7)
02623          LDQ  7)
02624          FMP  B
02625          STO  1)+1
02626          LDQ  SUM-4
02627          FMP  B-1
02630          STO  1)+2
02631          LDQ  SUM-3
02632          FMP  B
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02633           STO  1)+3
02634           LDQ  B-1
02635           FMP  B-1
02636           STO  1)+4
02637           LDQ  1)+4
02640           FMP  3)+1
02641           STO  7)
02642           LDQ  7)
02643           FMP  SUM-2
02644           STO  1)+5
02645           LDQ  B
02646           FMP  B
02647           STO  1)+6
02650           LDQ  1)+6
02651           FMP  3)+1
02652           STO  7)
02653           LDQ  7)
02654           FMP  SUM-1
02655           CHS
02656           FAD  CUE
02657           FSB  1)+5
02660           FAD  1)+3
02661           FAD  1)+2
02662           FAD  1)+1
02663           STO  C
02664  311A    CLA  C
02665           SXD  6)+4,4
02666           TSX  EXP,4
02667           NTR  *+2,0,35
02670           PZE  0,0,311
02671           LXD  6)+4,4
02672           STO  PH
02673  312A     LXD  2)+2,1
02674           CLA  N
02675           STD  315A2
02676           LXD  II,2
02677  313A     LDQ  Y+1,1
02700           FMP  SUM-5
02701           STO  7)
02702           LDQ  7)
02703           FMP  X+1,1
02704           STO  1)+1
02705           LDQ  SUM-4
02706           FMP  Y+1,1
02707           STO  1)+2
02710           LDQ  SUM-3
02711           FMP  X+1,1
02712           STO  1)+3
02713           LDQ  Y+1,1
02714           FMP  Y+1,1
02715           STO  1)+4
02716           LDQ  1)+4
02717           FMP  3)+1
02720           STO  7)
02721           LDQ  7)
02722           FMP  SUM-2
02723           STO  1)+5
02724           LDQ  X+1,1
02725           FMP  X+1,1
02726           STO  1)+6

02727           LDQ  1)+6
02730           FMP  3)+1
02731           STO  7)
02732           LDQ  7)
02733           FMP  SUM-1
02734           CHS
02735           FAD  SUM
02736           FSB  1)+5
02737           FAD  1)+3
02740           FAD  1)+2
02741           FAD  1)+1
02742           STO  CCUE+1,1
02743  314A     CLA  CCUE+1,1
02744           SXD  6)+4,4
02745           TSX  EXP,4
02746           NTR  *+2,0,35
02747           PZE  0,0,314
02750           LXD  6)+4,4
02751           STO  CCUE+1,1
02752  315A     CLA  RHO+1,2
02753           FSB  CCUE+1,1
02754           STO  DELTA+1,1
02755  315A1    TXI  *+1,1,1
02756           TXI  *+1,2,11
02757  315A2    TXL  313A,1
02760  316A     CLA  2)+4
02761           STO  L
02762           LXD  L,1
02763           SXD  C)G4,1
02764  317A     TRA  152A
02765  318A     CAL  *
02766           XIT  (LEV)
02767           ETM
02770           CAL  (IOH)0
02771           SLW  1
02772           CAL  (STH)
02773  318D1    NTR  8)3I,0,6
02774  319A     CAL  *
02775           XIT  (FIL)
02776  320A     CAL  *
02777           XIT  (LEV)
03000           ETM
03001           CAL  (IOH)0
03002           SLW  1
03003           CAL  (STH)
03004  320D1    NTR  8)3E,0,6
03005  321A     LXD  2)+2,2
03006  322A     ETM
03007           NTR  SUM+1,2
03010           LTM
03011  322A1    TXI  *+1,2,1
03012  322A2    TXL  322A,2,6
03013  324A     LTM
03014  325A     CAL  *
03015           XIT  (FIL)
03016  326A     TRA  173A
03017  2)       OCT  +000000000003
03020           OCT  +000011000000
03021           OCT  +000001000000
03022           OCT  +000002000000

03023           OCT  +000003000000
03024           OCT  +000012000000
03025           OCT  +000004000000
03026           OCT  +000006000000
03027           OCT  +000013000000
03030  3)       OCT  +000000000000
03031           OCT  +200400000000
03032           OCT  +205660000000
03033           OCT  +204440000000
03034           OCT  +203440000000
03035           OCT  +202600000000
03036           OCT  +205440000000
03037           OCT  +204600000000
03040           OCT  +201600000000
03041           OCT  +201400000000
03042           OCT  +203600000000
03043           OCT  +203400000000
03044  6)       OCT  +233000000000
03045           OCT  +000000077777
03046           OCT  +000000000000
03047           OCT  +000001000000
03050           OCT  +000000000000
03051           BCD  18,2I6)
03052  8)3U     BCD  1(  E12.
03053  8)3C     BCD  1(  H1)
03054           BCD  16)
03055  8)3P     BCD  1(  H0,A
03056           BCD  1A6)
03057  8)3N     BCD  1(6X,11
03060           BCD  1NATES)
03061           BCD  1COORDI
03062           BCD  1  CELL
03063           BCD  10 UNIT
03064           BCD  1CTED T
03065           BCD  1 CORRE
03066           BCD  1INATES
03067           BCD  1 COORD
03070           BCD  1Z, MAP
03071           BCD  17HX,Y,
03072  8)3M     BCD  1(  H0,5
03073           BCD  1.6)
03074           BCD  1X,2F12
03075           BCD  112.0,3
03076  8)3L     BCD  1(3I6,F
03077           BCD  1IGHT)
03100           BCD  1EAK HE
03101  8)3K     BCD  1(  2H0P
03102           BCD  1     )
03103           BCD  1
03104           BCD  1
03105           BCD  1
03106           BCD  1
03107           BCD  1
03110           BCD  1
03111           BCD  1
03112           BCD  1
03113           BCD  1
03114           BCD  1
03115           BCD  1
03116  8)3J     BCD  1(72H
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03117            BCD  1,1HN)
03120            BCD  11HV11X
03121            BCD  1HU11X,
03122            BCD  1S11X,1
03123            BCD  111X,1H
03124            BCD  11X,1HR
03125            BCD  1X,1HP1
03126  8)3I      BCD  1(1H014
03127            BCD  1,1HM)
03130            BCD  11HW11X
03131            BCD  1HU11X,
03132            BCD  1T11X,1
03133            BCD  111X,1H
03134            BCD  11X,1HR
03135            BCD  1X,1HP1
03136  8)3H      BCD  1(1H014
03137            BCD  1,1HL)
03140            BCD  11HW11X
03141            BCD  1HV11X,
03142            BCD  1T11X,1
03143            BCD  111X,1H
03144            BCD  11X,1HS
03145            BCD  1X,1HP1
03146  8)3G      BCD  1(1H014
03147            BCD  18)
03150  8)3F      BCD  1(3F20.
03151            BCD  112.8)
03152  8)3E      BCD  1(8X,6F
03153            BCD  11HN)
03154            BCD  1HM11X,
03155            BCD  1L11X,1
03156            BCD  111X,1H
03157            BCD  11X,1HW
03160            BCD  1X,1HV1
03161  8)3D      BCD  1(1H014
03162            BCD  13.8)
03163  8)V7      BCD  1(7X,F1
03164            BCD  11HU)
03165            BCD  1HT11X,
03166            BCD  1S11X,1
03167            BCD  111X,1H
03170            BCD  11X,1HR
03171            BCD  1X,1HP1
03172  8)3C      BCD  1(1H014
03173            BCD  10)
03174            BCD  1,11F6.
03175  8)3A      BCD  1(3F2.0
03176            BCD  1F6.0)
03177  8)39      BCD  1(6X,11
03200            BCD  1NATES)
03201            BCD  1COORDI
03202            BCD  1O MAP
03203            BCD  1CTED T
03204            BCD  1 CORRE
03205            BCD  1VALUES
03206            BCD  1,Y,Z,
03207  8)38      BCD  1(43H0X
03210            BCD  1/)
03211            BCD  1A RHO/
03212            BCD  19HDELT
03213            BCD  1
03214            BCD  1
03215            BCD  1LC5X,
03216            BCD  1RHO CA
03217            BCD  106X,8H
03220            BCD  1X,3HRH
03221            BCD  1X,1HZ8
03222            BCD  1X,1HY5
03223            BCD  1X,1HX5
03224  8)36      BCD  1(/1H04
03225            BCD  1)
03226            BCD  1704F//
03227            BCD  1CHINE
03230            BCD  1E2. MA
03231            BCD  1 CODE
03232            BCD  1T 146,
03233            BCD  1552/ME
03234            BCD  1ITLE 1
03235  8)34      BCD  1(42H1T
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ACKNOWLEDGMENT

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REFERENCES

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APPENDIX

Procedure: The general least-squares method requires that values of the parameters be found such that

$$\sum_{i=1}^{N} E_i^2 = \sum_{i=1}^{N} \left(p - \frac{r}{2} x_i^2 - \frac{s}{2} y_i^2 - \frac{t}{2} z_i^2 + ux_i + vy_i + wz_i + ly_iz_i + mx_iz_i + nx_iy_i - \ln \rho_i \right)^2$$

will be a minimum.

By differentiating with respect to each of the ten parameters (6 in the two-dimensional case), the normal equations are obtained:

$$\frac{\partial \Sigma E_i^2}{\partial \rho} = \sum_{i=1}^{N} (E_i) = 0 \quad , \tag{1}$$

$$\frac{\partial \Sigma E_i^2}{\partial r} = \sum_{i=1}^{N} (E_i)(-x_i^2/2) = 0 \quad , \tag{2}$$

$$\frac{\partial \Sigma E_i^2}{\partial s} = \sum_{i=1}^{N} (E_i)(-y_i^2/2) = 0 \quad , \tag{3}$$

$$\frac{\partial \Sigma E_i^2}{\partial t} = \sum_{i=1}^{N} (E_i)(-z_i^2/2) = 0 \quad , \tag{4}$$

$$\frac{\partial \Sigma E_i^2}{\partial u} = \sum_{i=1}^{N} (E_i)(x_i) = 0 \quad , \tag{5}$$

$$\frac{\partial \Sigma E_i^2}{\partial v} = \sum_{i=1}^{N} (E_i)(y_i) = 0 \quad , \tag{6}$$

$$\frac{\partial \Sigma E_i^2}{\partial w} = \sum_{i=1}^{N} (E_i)(z_i) = 0 \quad , \tag{7}$$

$$\frac{\partial \Sigma E_i^2}{\partial l} = \sum_{i=1}^{N} (E_i)(y_iz_i) = 0 \quad , \tag{8}$$

$$\frac{\partial \Sigma E_i^2}{\partial m} = \sum_{i=1}^{N} (E_i)(x_i z_i) = 0 \quad , \tag{9}$$

$$\frac{\partial \Sigma E_i^2}{\partial n} = \sum_{i=1}^{N} (E_i)(x_i y_i) = 0 \quad . \tag{10}$$

Evaluation of the equations at the N points results in a system of linear equations unknown in the parameters. The system is solved by matrix inversion subroutine AN F402.

The partial derivatives of $\ln\rho$ with respect to x, y, and z result in a system of linear equations after equating each to zero:

$$\frac{\partial \ln\rho}{\partial x} = -rx + u + mz + ny = 0 \quad , \tag{1}$$

$$\frac{\partial \ln\rho}{\partial y} = -sy + v + lz + nx = 0 \quad , \tag{2}$$

$$\frac{\partial \ln\rho}{\partial z} = -tz + w + ly + mx = 0 \quad . \tag{3}$$

By replacing the parameters by their previously calculated values and once again utilizing AN F402, values of x, y, and z are found.

Coordinates of the peak corrected to map coordinates are found merely by adding algebraically the computed values of x, y, and z to their corresponding values at the origin of the initial array.

Coordinates of the peak corrected to unit-cell coordinates are found by multiplying the x, y, and z map coordinates by DX, DY, and DZ, respectively.

The peak height is computed by substituting the calculated values of x, y, and z and the values of the parameters into the initial equation representing the peak.