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Argonne National Laboratory

PROGRAM FOR THE LOCATION OF FOURIER PEAK CENTERS

by

M. H. Mueller, Fred Clark,
and S. H. Simonsen

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PROGRAM FOR THE LOCATION OF FOURIER PEAK CENTERS

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The University of Texas

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	X coordinate, 2nd case.
		etc.	
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	Y coordinate, 1st case.
		etc.	
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	Z coordinate, 1st case.
		etc.	
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 II

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								
.00	833333	.00	833333	.01	666667	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

Figure 1 (Continued)

COST CODE 1552

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,F13.8)
  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 COORDINATES 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   )
```

ANL-30

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 LOCATIONS 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

```
00000 EXP      BCD 1EXP
00001 MATINV   BCD 1MATINV
00002 LOG      BCD 1LOG
00003 (FIL)    BCD 1(FIL)
00004 (STH)    BCD 1(STH)
00005 (IOH)O   BCD 1(IOH)O
00006 (RTN)    BCD 1(RTN)
00007 (TSH)    BCD 1(TSH)
00010 (IOH)I   BCD 1(IOH)I
00011 (LEV)    BCD 1(LEV)
00012 23A      CAL *
00013          XIT (LEV)
00014          ETM
00015          CAL (IOH)I
00016          SLW 1
00017          CAL (TSH)
00020 23D1     NTR 8)3J,0,7
00021 24A      CAL *
00022          XIT (RTN)
00023 25A      CAL *
00024          XIT (LEV)
00025          ETM
00026          CAL (IOH)I
00027          SLW 1
00030          CAL (TSH)
00031 25D1     NTR 8)3U,0,7
00032 26A      ETM
00033          NTR SFX
00034          NTR SFY
00035          NTR SFZ
00036          NTR K
00037          NTR N
00040          LTM
00041 27A      CAL *
00042          XIT (RTN)
00043 28A      CAL *
00044          XIT (LEV)
00045          ETM
00046          CAL (IOH)I
00047          SLW 1
00050          CAL (TSH)
00051 28D1     NTR 8)39,0,7
00052 29A      LXD 2)+2,2
00053          CLA K
00054          STD 30A2
00055 30A      ETM
00056          NTR R+1,2
00057          LTM
00060 30A1     TXI *+1,2,1
00061 30A2     TXL 30A,2
00062 32A      LTM
00063 33A      CAL *
00064          XIT (RTN)
00065 34A      CAL *
00066          XIT (LEV)
00067          ETM
00070          CAL (IOH)I
00071          SLW 1
00072          CAL (TSH)
00073 34D1     NTR 8)39,0,7
00074 35A      LXD 2)+2,2
00075          CLA K
00076          STD 36A2
00077 36A      ETM
00100          NTR R-9,2
00101          LTM
00102 36A1     TXI *+1,2,1
00103 36A2     TXL 36A,2
00104 38A      LTM
00105 39A      CAL *
00106          XIT (RTN)
00107 40A      CAL *
00110          XIT (LEV)
00111          ETM
00112          CAL (IOH)I
00113          SLW 1
00114          CAL (TSH)
00115 40D1     NTR 8)39,0,7
00116 41A      LXD 2)+2,2
00117          CLA K
00120          STD 42A2
00121 42A      ETM
00122          NTR R-19,2
00123          LTM
00124 42A1     TXI *+1,2,1
00125 42A2     TXL 42A,2
00126 44A      LTM
00127 45A      CAL *
00130          XIT (RTN)
00131 46A      CAL *
00132          XIT (LEV)
00133          ETM
00134          CAL (IOH)I
00135          SLW 1
00136          CAL (TSH)
00137 46D1     NTR 8)3N,0,7
00140 47A      LXD 2)+2,2
00141          CLA K
00142          STD 48A2
00143 48A      ETM
00144          NTR AA+1,2
00145          LTM
00146 48A1     TXI *+1,2,1
00147 48A2     TXL 48A,2
00150 50A      LTM
00151 51A      CAL *
00152          XIT (RTN)
00153 52A      CAL *
00154          XIT (LEV)
00155          ETM
00156          CAL (IOH)O
00157          SLW 1
00160          CAL (STH)
00161 52D1     NTR 8)34,0,6
00162 53A      CAL *
00163          XIT (FIL)
00164 54A      CAL *
00165          XIT (LEV)
00166          ETM
00167          CAL (IOH)O
00170          SLW 1
00171          CAL (STH)
00172 54D1     NTR 8)3J,0,6
00173 55A      CAL *
00174          XIT (FIL)
00175 56A      LXD 2)+2,2
00176          CLA K
00177          STD 60A2
00200          CLA K
00201          SUB 6)+3
00202          STD 63A3
00203          ADD 2)+8
00204          STD 63A1
00205          CLA K
00206          STD 60A3
00207          LXD 2)+2,4
00210          CLA N
00211          STD 63A4
00212 57A      CAL *
00213          XIT (LEV)
00214          ETM
00215          CAL (IOH)I
00216          SLW 1
00217          CAL (TSH)
00220 57D1     NTR 8)3A,0,7
00221 58A      ETM
00222          NTR X+1,4
00223          NTR Y+1,4
00224          NTR Z+1,4
00225          LTM
       59A     BSS
00226 60A      ETM
00227          NTR RHO+1,2
00230          LTM
00231 60A1     TXI *+1,2,1
00232 60A2     TXL 60A,2
00233 60A3     TIX 60A3+1,2
00234 62A      LTM
00235 63A      CAL *
00236          XIT (RTN)
00237 63A1     TXI 63A1+1,2
00240          SXD 60A2,2
00241 63A3     TIX 63A3+1,2
00242          TXI *+1,4,1
00243 63A4     TXL 57A,4
00244 64A      CLA 2)
00245          STO II
00246          LXD II,2
00247          SXD C)G2,2
00250          LXD II,4
00251          SXD C)106,4
00252 65A      CLA N
00253          SUB 2)+1
00254 65A1     TZE 66A
00255          TPL 81A
00256          TRA 81A
00257 66A      CLA 3)
00260          STO TOT1
00261 67A      LXD 2)+2,4
00262          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 73A2
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 101A     STZ A+1,1
00512 101A1    TXI *+1,1,20
00513 101A2    TXL 101A,1,400
00514 101A3    TIX 101A3+1,1,400
00515 101A4    TXI *+1,1,1
00516 101A5    TXL 101A,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-1
00525 105A     CLA 3)+3
00526          STO A-
00527 106A     CLS 3)+3
00530          STO A-10
00531 107A     CLS 3)+4
00532          STO A-11
00533 108A     CLS 3)+5
00534          STO A-12
00535 109A     CLS 3)+5
00536          STO A-23
00537 110A     CLS 3)+3
00540          STO A-40
00541 111A     CLS 3)+5
00542          STO A-41
00543 112A     CLS 3)+4
00544          STO A-42
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 151A2
01000          LXD II,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  *+2,0,16
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  II,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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01314          XIT (LEV)
01315          ETM
01316          CAL (IOH)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-20
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 233A2
01541 233A     STZ SUM+1,1
01542 233A1    TXI *+1,1,1
01543 233A2    TXL 233A,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 0,0,238
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 255A2
01774          LXD II,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 *+2,0,26
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 *+1,1,1
02054          TXI *+1,2,11
02055  255A2   TXL 253A,1
02056  256A    CLA 2)+2
02057          STO L
02060          LXD L,
02061          SXD C)G4,1
02062  257A    TRA 152A
```

```
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-2
02257 280A    LDQ B-2
02260         FMP SUM-5
02261         STO 7)
02262         LDQ 7)
02263         FMP B
02264         STO 1)+1
02265         LDQ SUM-4
02266         FMP B-2
02267         STO 1)+2
02270         LDQ SUM-3
02271         FMP B
02272         STO 1)+3
02273         LDQ B-2
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
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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 +000000000000
03020          OCT +000011000000
03021          OCT +000001000000
03022          OCT +000002000000
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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 18,216)
03052 8)3U     BCD 1(3E12.
03053 8)3Q     BCD 1(1H1)
03054          BCD 16)
03055 8)3P     BCD 1(1H0,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(1H0,5
03073          BCD 1.6)
03074          BCD 1X,2F12
03075          BCD 112.0,3
03076 8)3L     BCD 1(3I6,F
03077          BCD 11GHT)
03100          BCD 1EAK HE
03101 8)3K     BCD 1(12HOP
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 10 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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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.

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