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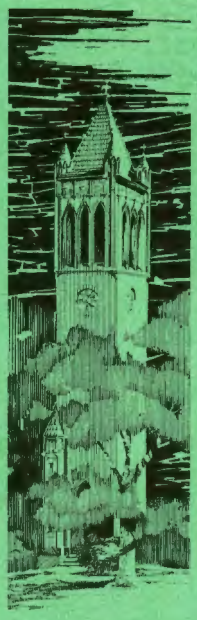
Disciplines
Computer Sciences | Mathematics



IOWA STATE UNIVERSITY

ORIGIN IMAGE SEEKER, AN IMAGE SEEKING PROGRAM FOR PATTERSON PROJECTIONS AND HARKER SECTIONS

by

D. A. Hansen and D. H. Erbeck

AMES LABORATORY

RESEARCH AND DEVELOPMENT REPORT

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ABSTRACT

Origin Image Seeker is a program for the IBM-7074. It is written in Fortran, although the program uses an Autocoder subroutine. This program determines trial structures from Patterson projections and Harker sections provided that the projection contains either a real or projected atom at the origin or that the section contains a real atom at the origin.

INTRODUCTION

If one considers a unit cell having an atom at the origin, then it follows that any Patterson projection characterizing the structure will contain maxima corresponding to atomic positions. The same is true for any Harker section with an atom at the origin. For structures having atoms in axial positions, but not having an atom at the origin, the appropriate Patterson projection will still have a projected atom at the origin. Under these conditions, some of the maxima correspond to atomic positions, and hence, it is possible to extract self-consistent trial structures from Patterson projections or from Harker sections.

DISCUSSION

The most general case of a projected atom at the origin will be treated. In this case, it will be assumed that the Patterson projection is $P(x, y, 0)$. If two given peaks, A at $(x_1, y_1, 0)$ and B at $(x_2, y_2, 0)$,

are both atomic positions, then their difference, A-B at $(x_1-x_2,\ y_1-y_2,\ 0)$, must exist in the appropriate position in the projection, provided that the peak multiplicity is adequate. In this case, A and B constitute a "possible" pair. If the difference between A and B does not appear in the projection, at least one of the peaks is not an atomic position and the pair is "impossible". One purpose of the Fortran section of Origin Image Seeker is to generate a list of the possible pairs.

Once the possible pair list is generated, the list is searched in order to determine which of the Patterson peaks occurs least often as an "interset" (the difference between two other peaks) vector; this peak is defined as a "basis vector" which must correspond either to an atomic position or to the difference between two atomic positions. The Finder subroutine determines both the basis vectors and the possible pairs whose difference corresponds to the basis vectors.

If one assumes that the basis vector corresponds to an atomic position, then a trial structure is generated by merely determining which of the other Patterson peaks combine with the basis vector to form a self-consistent possible pair list. Each peak in the self-consistent possible pair list combined with any other peak in this list generates a peak appearing in the projection.

If one assumes that the basis vector does not correspond to an atomic position, then it must correspond to the difference of a possible pair. In this case, a trial structure is generated by determining a self-consistent list of Patterson peaks which form possible pairs with each member of the possible pair which generated the basis vector.

Since there may be a number of peaks which occur least often as an interset vector in the possible pair list, there may be more than one trial structure of the type generated by assuming the basis vector to be an atomic position. Similarly, there may be a number of possible pairs whose difference corresponds to a given basis vector and hence, there may be more than one trial structure of this type for each basis vector.

The Finder subroutine is responsible for generating the trial structures. The remainder of the Fortran section of the program prints the output from the Finder subroutine.

INTERPRETATION OF OUTPUT

After the list of Patterson peaks is read as input data, each peak is given a number and is thereafter referred to in terms of this number. The output listing of the Patterson peaks and trial structures is characterized by the use of these peak numbers.

Examination of the sample output listing shows that a given basis vector and its associated trial structure is listed. Then, under right-handed indentation, the possible pairs capable of generating the given basis vector, along with their associated trial structures, are listed. The members A and B of the possible pairs responsible for the generation of a given basis vector are listed under the labels "the basis vectors are I = A and J = B". Note that every basis vector is a member of the trial structure with which it is listed.

In order to select the most probable trial structure from the output, the following procedure is recommended. Since, if the input peaks are

complete and correct, there is at least one correct trial structure for each basis vector, choose the most likely trial structure as the one that occurs most often in the list of trial structures. This procedure may fail if the input data are either incomplete or inaccurate.

Most Patterson projections lack the resolution necessary to ensure that all of the observed maxima correspond to either atomic positions or interatomic vectors. Hence it is quite possible to obtain either incomplete or, in the worst cases, completely spurious trial structures. In the latter case, the image seeking function may select a spurious peak as a basis vector. In this case, all of the trial structures generated for this basis vector will be wrong. Hence, one should determine whether the basis vectors correspond to sharply defined peaks. If the user has little confidence in these peaks, he may bias the basis vector selection by increasing the number of Patterson peaks in the input list. These additional peaks must correspond to the possible pairs whose differences generate the peaks which the user wishes to eliminate as basis vectors. The user may also eliminate the questionable peaks from the input list.

If the user suspects that a trial structure is incomplete, he should select the most likely space group and generate trial structures, using the incomplete trial structure parameters and the space group atomic positions. Comparison of these user-generated trial structures with the Patterson projection may indicate areas of "wash-out" which correspond to the missing maxima.

Finally, if the positional uncertainties, Δx and Δy are too large, the correct trial structure may be accompanied by a list of non-atomic

peaks. Since there is no way for the user to determine the minimum error without extensive calculation, the following method is recommended as standard procedure: select what appears to be a reasonable error and run successive Patterson decks with errors of decreasing magnitude. Examination of the resulting output lists will indicate which of the peaks (forming the original trial structure) may be non-atomic peaks.

In the event that a given Patterson peak A does not correspond to an interset peak, the following message is printed: "peak A has zero multiplicity in the possible pair list." This can happen for one of two reasons: (1) the entire projection was not used and (2), the peak corresponds to neither an atomic peak nor an interset peak. In the former case, if less than the whole projection is used as input data (normally because there are more than 150 peaks in the complete projection), the peaks characterized by the largest values of x, y, or z cannot be generated as interset vectors, even though they may correspond to valid maxima. In this case, the message should be ignored. However, if the peak does not have a maximum x, y, or z, it is probably a spurious peak. If examination of the projection causes the user to place little confidence in this peak, he should eliminate the peak from the input list and resubmit the resulting deck.

If the complete Patterson projection was used as input data, a peak of zero multiplicity usually corresponds to a spurious maximum. An examination of the projection should show whether or not this peak is spurious. If the user concludes that the peak is spurious, he should remove it from the input list and resubmit the deck.

OPERATOR INSTRUCTIONS

Card 1 FORMAT(I3)

NPROB, the number of different Patterson projections in this job.

Note: A set of the following cards must be included for each projection in this job.

Card 2 FORMAT(72H)

Put in any 71 character title with a 1 in column 1.

Card 3 FORMAT(I3)

Punch a 1 in column 3 for a P(x, y) Patterson projection.

Punch a 2 in column 3 for a P(x, z) Patterson projection.

Punch a 3 in column 3 for a P(y, z) Patterson projection.

Card 4 FORMAT(I3)

NP, the number of Patterson peaks to be used as input data. $0 \leq NP \leq 150$.

Card 5 FORMAT(2F5.3)

Δx and Δy, the positional uncertainties common to all peaks. Keep Δx and Δy as small as possible, since large values imply a lack of resolution in the projection.

Data Cards FORMAT(2F5.3)

One card is punched for each peak, x being punched in columns 1 through 5 and y being punched in columns 6 through 10. There should be NP of these cards. Note that the program reads the position of the peak as if it were from a P(x, y) projection, even if the data correspond to P(x, z) or P(y, z) projections.

C FOR COMMENT

STATEMENT NUMBER 1–5	Cont. 6	FORTRAN STATEMENT 7–72
1		
1 NI3SN4 IDEAL TEST DATA		
2		
49		
0.0130	0	.013
0.0720	0	.325
0.1800	0	.800
0.4280	0	.675
0.3200	0	.200
0.2800	0	.650
0.2200	0	.350
0.5000	0	.000
0.9280	0	.675
0.8200	0	.200
0.5720	0	.325
0.6800	0	.800
0.7200	0	.350
0.7800	0	.650
0.1080	0	.475
0.1480	0	.025
0.2080	0	.325

C FOR COMMENT

STATEMENT NUMBER 1 5	Cont. 6	FORTRAN STATEMENT 7 72
0.4400	0	.700
0.3600	0	.600
0.4000	0	.150
0.4600	0	.450
0.1440	0	.650
0.2520	0	.125
0.2920	0	.675
0.3520	0	.975
0.3920	0	.525
0.0600	0	.300
0.1400	0	.400
0.1000	0	.850
0.0400	0	.550
0.3560	0	.350
0.2480	0	.875
0.8920	0	.525
0.8520	0	.975
0.7920	0	.675
0.5600	0	.300
0.6400	0	.400
0.6000	0	.850

C FOR COMMENT

STATEMENT NUMBER (1–5)	Cont. (6)	FORTRAN STATEMENT (7–72)
0.540	0	.550
0.856	0	.350
0.748	0	.875
0.708	0	.325
0.648	0	.025
0.608	0	.475
0.940	0	.700
0.860	0	.600
0.900	0	.150
0.960	0	.450
0.644	0	.650
0.752	0	.125

SAMPLE OUTPUT

NI3SN4 IDEAL TEST DATA
NUMBER OF PATTERSON PEAKS IS 49
PATTERSON PEAK INPUT

X	Z	I
0.072	0.325	1
0.180	0.800	2
0.428	0.675	3
0.320	0.200	4
0.280	0.650	5
0.220	0.350	6
0.500	0.000	7
0.928	0.675	8
0.820	0.200	9
0.572	0.325	10
0.680	0.800	11
0.720	0.350	12
0.780	0.650	13
0.108	0.475	14
0.148	0.025	15
0.208	0.325	16
0.440	0.700	17
0.360	0.600	18
0.400	0.150	19
0.460	0.450	20
0.144	0.650	21
0.252	0.125	22
0.292	0.675	23
0.352	0.975	24
0.392	0.525	25
0.060	0.300	26
0.140	0.400	27
0.100	0.850	28
0.040	0.550	29
0.356	0.350	30
0.248	0.875	31
0.892	0.525	32
0.852	0.975	33
0.792	0.675	34
0.560	0.300	35
0.640	0.400	36
0.600	0.850	37
0.540	0.550	38
0.856	0.350	39
0.748	0.875	40
0.708	0.325	41
0.648	0.025	42
0.608	0.475	43
0.940	0.700	44
0.860	0.600	45
0.900	0.150	46
0.960	0.450	47
0.644	0.650	48
0.752	0.125	49

```
BASIS VECTOR IS 17
   TRIAL STRUCTURE 1
   NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 7
      ATOMIC POSITIONS     I
                           6
                           7
                          12
                          15
                          19

          BASIS VECTORS ARE I = 12 AND J = 5
          TRIAL STRUCTURE 2
          NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 14
             ATOMIC POSITIONS     I
                                  1
                                  2
                                  3
                                  4
                                  6
                                  7
                                  8
                                  9
                                 10
                                 11
                                 13

          BASIS VECTORS ARE I = 34 AND J = 24
          TRIAL STRUCTURE 3
          NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 14
             ATOMIC POSITIONS     I
                                  1
                                  7
                                 10
                                 21
                                 22
                                 23
                                 25
                                 32
                                 33
                                 48
                                 49

          BASIS VECTORS ARE I = 38 AND J = 28
          TRIAL STRUCTURE 4
          NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 14
             ATOMIC POSITIONS     I
                                  4
                                  7
                                  9
                                 25
                                 27
                                 29
                                 31
                                 32
                                 36
                                 37
                                 40
```

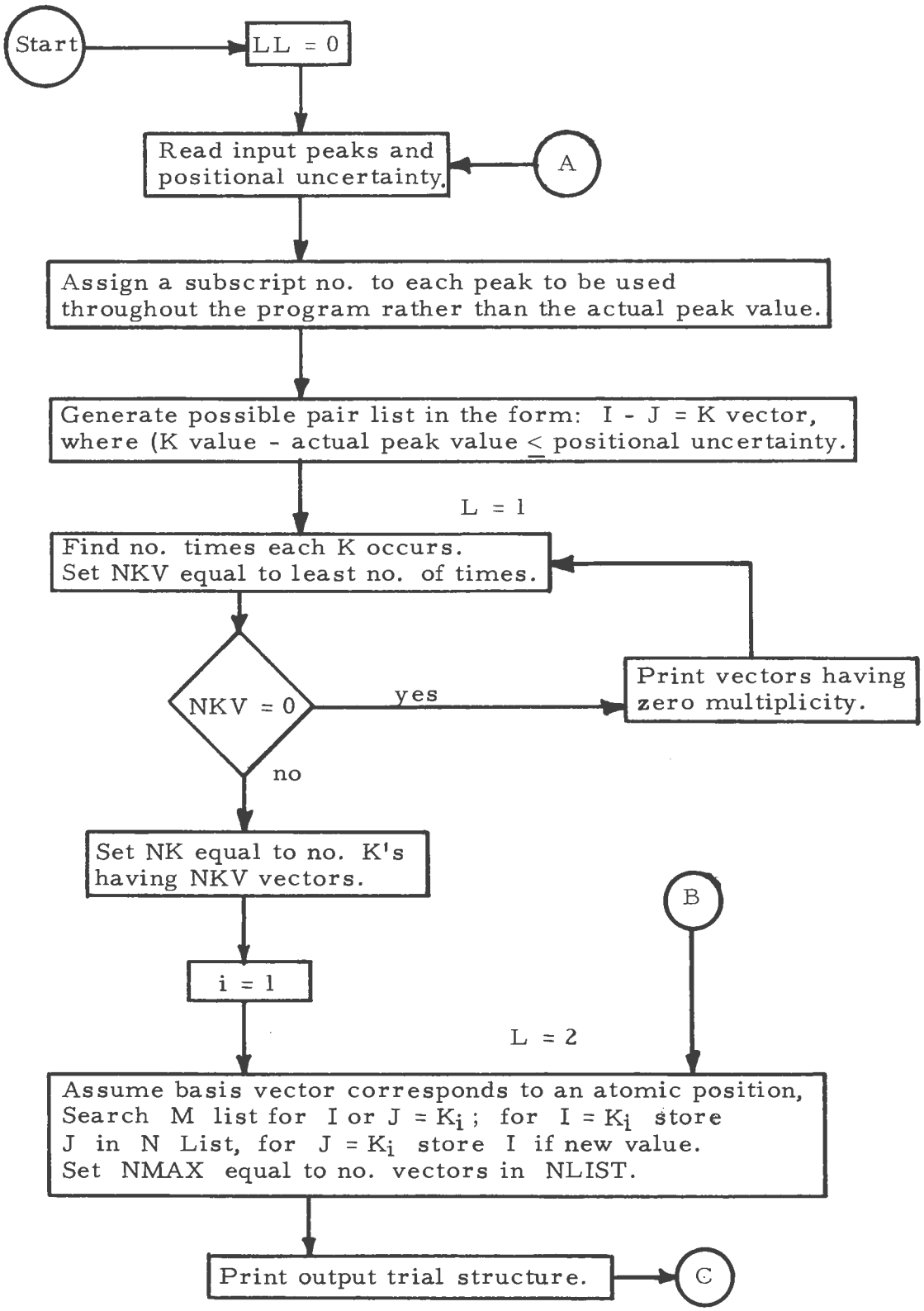
BASIS VECTORS ARE I = 42 AND J = 16
TRIAL STRUCTURE 5
NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 14
ATOMIC POSITIONS I
3
7
8
14
15
30
31
39
40
41
43

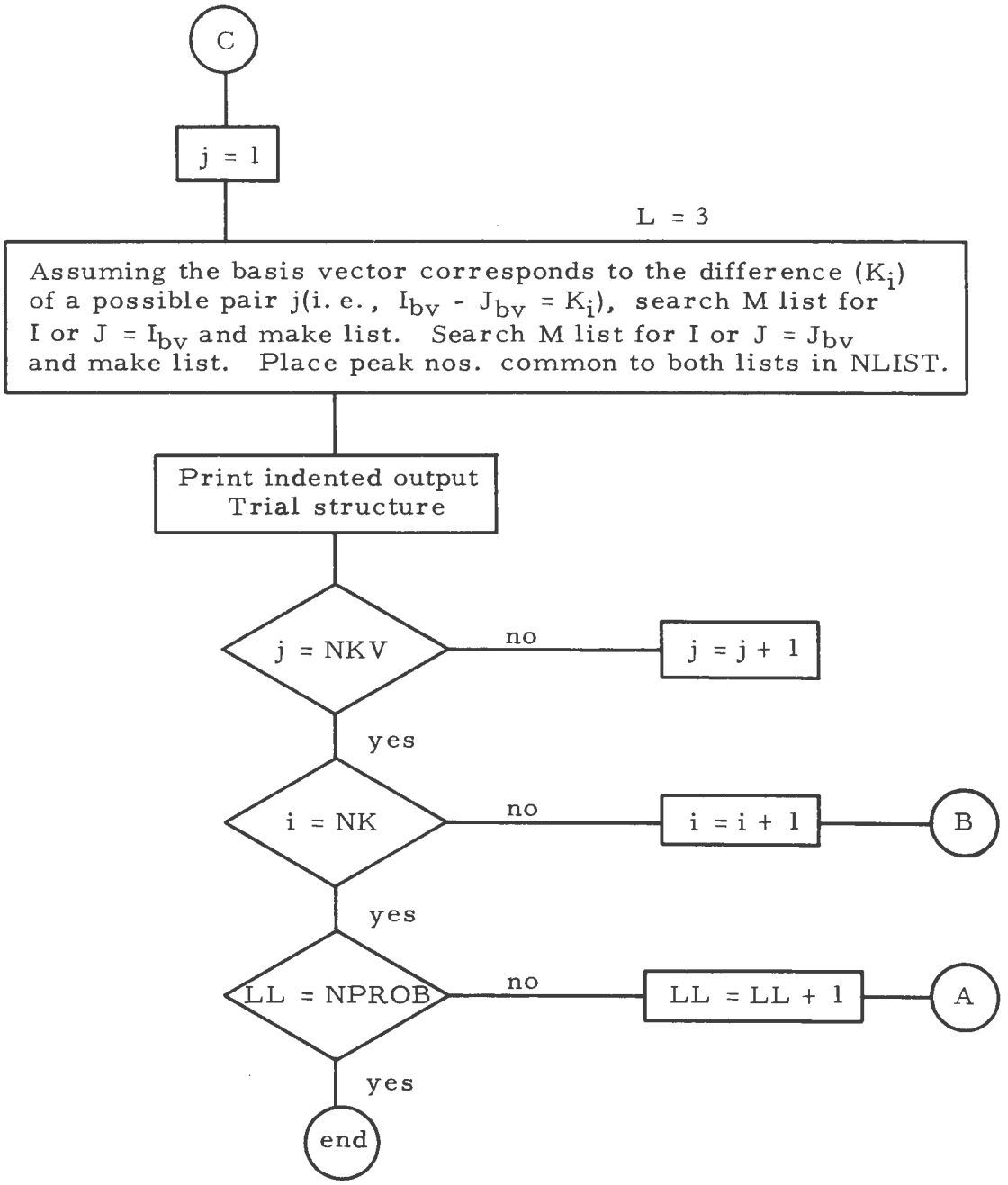
BASIS VECTORS ARE I = 44 AND J = 7
TRIAL STRUCTURE 6
NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 14
ATOMIC POSITIONS I
6
12
15
17
19
23
29
34
38
42
46

BASIS VECTORS ARE I = 46 AND J = 20
TRIAL STRUCTURE 7
NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS 14
ATOMIC POSITIONS I
2
7
11
14
18
19
22
43
45
47
49

```
BASIS VECTOR IS  18
   TRIAL STRUCTURE IS  8
   NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS  7
      ATOMIC POSITIONS     1
                           2
                           7
                          11
                          14
                          19
```

Note: For the sake of brevity, the remaining 76 trial structures listed in the output are omitted. The correct trial structure is trial structure number 2. One must remember that every basis vector is a member of the trial structure with which it is listed.


Start
LL = 0
Read input peaks and positional uncertainty.
A
Assign a subscript no. to each peak to be used throughout the program rather than the actual peak value.
Generate possible pair list in the form: I - J = K vector, where (K value - actual peak value ≤ positional uncertainty.
L = 1
Find no. times each K occurs. Set NKV equal to least no. of times.
NKV = 0
yes
Print vectors having zero multiplicity.
no
Set NK equal to no. K's having NKV vectors.
B
i = 1
L = 2
Assume basis vector corresponds to an atomic position, Search M list for I or J = K_i ; for I = K_i store J in N List, for J = K_i store I if new value. Set NMAX equal to no. vectors in NLIST.
Print output trial structure.
C


C
j = 1
L = 3
Assuming the basis vector corresponds to the difference (K_i) of a possible pair j(i. e., I_{bv} - J_{bv} = K_i), search M list for I or J = I_{bv} and make list. Search M list for I or J = J_{bv} and make list. Place peak nos. common to both lists in NLIST.
Print indented output Trial structure
j = NKV
no
j = j + 1
yes
i = NK
no
i = i + 1
B
yes
LL = NPROB
no
LL = LL + 1
A
yes
end

The flow diagram is intended only to show the logic involved, not the exact relationship between the main routine, Seeker, and the subroutine, Finder. Most of the logical computation is done in Finder in blocks marked L = 1, 2 or 3 on the flow chart; Seeker takes care of the house keeping and I/O.

Parameter	Refers to
L	which section (1, 2 or 3) of the subroutine is being called by the main routine
M	the input possible pair list of vectors generated by the main routine
N	the no. of vectors in M
NK	the no. of K's having NKV vectors
NMAX	the no. of peaks in NLIST
NLIST	the list of peak nos. chosen to return
IBV	the subscript no. of basis vector I_{bv}
JBV	the subscript no. of basis vector J_{bv}
K	the subscript no. of basis vector K

ACKNOWLEDGMENTS

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```
C      ORIGIN IMAGE SEEKER
       DIMENSION X(150),Y(150),M(9999),NLIST(150)
       COMMON M
 1000 FORMAT (1H1)
 1001 FORMAT (72H
     1                    )
 1002 FORMAT (2I3)
 1003 FORMAT (2F5.3)
 1010 FORMAT (29H NUMBER OF PATTERSON PEAKS IS,I3)
 1011 FORMAT (21H PATTERSON PEAK INPUT)
 1012 FORMAT (3X2H X,6X1HY,6X1HI)
 1013 FORMAT (2XF5.3,2XF5.3,2XI3)
 1014 FORMAT (///16H BASIS VECTOR IS,I3)
 1015 FORMAT (2X16H TRIAL STRUCTURE,I3)
 1016 FORMAT (4X21H ATOMIC POSITIONS   I)
 1017 FORMAT (22XI3)
 1018 FORMAT (//8X21H BASIS VECTORS ARE I=,I3,7H AND J=,I3)
 1019 FORMAT (8X16H TRIAL STRUCTURE,I3)
 1020 FORMAT (10X21H ATOMIC POSITIONS   I)
 1021 FORMAT (28XI3)
 1022 FORMAT (5H PEAK,I3,48H HAS ZERO MULTIPLICITY IN THE POSSIBLE PAIR
     1LIST)
 1023 FORMAT (2X43H NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS,I3)
 1024 FORMAT (8X43H NUMBER OF ATOMS IN THIS TRIAL STRUCTURE IS,I3)
 1025 FORMAT (3X2H X,6X1HZ,6X1HI)
 1026 FORMAT (3X2H Y,6X1HZ,6X1HI)
       READ 1002,NPROB
C      NPROB IS THE NUMBER OF DATA DECKS IN THIS RUN.
C      NPROB IS NOT TO EXCEED 999.
       DO 110 LL=1,NPROB
       PRINT 1000
       READ 1001
       PRINT 1001
       READ 1002,NDATA
C      NDATA IS 1 FOR A P(X,Y) PATTERSON.
C      NDATA IS 2 FOR A P(X,Z) PATTERSON.
C      NDATA IS 3 FOR A P(Y,Z) PATTERSON.
       READ 1002,NP
C      NP IS THE TOTAL NUMBER OF PATTERSON PEAKS TO BE USED AS INPUT.
C      NP IS NOT TO EXCEED 150.
       PRINT 1010,NP
       PRINT 1011
       GO TO (1,2,3),NDATA
     1 PRINT 1012
       GO TO 9
     2 PRINT 1025
       GO TO 9
     3 PRINT 1026
     9 READ 1003,DX,DY
C      DX AND DY ARE THE POSITIONAL UNCERTAINTIES COMMON TO ALL PEAKS.
       DO 10 I=1,NP
       READ 1003,XX,YY
       X(I)=XX
       Y(I)=YY
    10 PRINT 1013,XX,YY,I
       N=0
       DO 22 I=2,NP
       IK=I-1
        DO 21 J=1,IK
         DO 20 K=1,NP
         XC=X(I)-X(J)
         IF(XC)11,13,12
    11   XC=XC+1.0
```

```
22          12    IF(ABSF(X(K)-XC)-DX)13,13,20
            13    YC=Y(I)-Y(J)
                  IF(YC)14,15,15
            14    YC=YC+1.0
            15    IF(ABSF(Y(K)-YC)-DY)16,16,20
            16    N=N+1
                  M(N)=K+1000*J+1000000*I
            20    CONTINUE
            21   CONTINUE
            22 CONTINUE
          C      START IMAGE SEEKING
                 L=1
                 CALL FINDER(L,M,N,NK,NKV,NMAX,NLIST,IBV,JBV,NP,K)
                 IF(NMAX-1)27,25,25
            25 DO 26 J=1,NMAX
            26 PRINT 1022,NLIST(J)
            27 M1=1
                 DO 100 I=1,NK
                 NKV1=NKV+1
                  DO 90 J=1,NKV1
                  IF(J-1)30,30,40
            30   L=2
                  GO TO 41
            40   L=3
            41 CALL FINDER(L,M,N,I,NKV,NMAX,NLIST,IBV,JBV,NP,K)
                 IF(NMAX-1)42,45,45
            42 IF(L-2)43,43,44
            43 PRINT 1014,K
                 PRINT 1015,M1
                 NPMAX=2
                 PRINT 1023,NPMAX
                 M1=M1+1
                 GO TO 90
            44 PRINT 1018,IBV,JBV
                 PRINT 1019,M1
                 NPMAX=3
                 PRINT 1024,NPMAX
                 M1=M1+1
                 GO TO 90
            45 IF(L-2)50,50,60
            50 PRINT 1014,K
                 PRINT 1015,M1
                 NPMAX=NMAX+2
                 PRINT 1023,NPMAX
                 PRINT 1016
                 M1=M1+1
                 DO 55 JJ=1,NMAX
            55 PRINT 1017,NLIST(JJ)
                 GO TO 90
            60 PRINT 1018,IBV,JBV
                 PRINT 1019,M1
                 NPMAX=NMAX+3
                 PRINT 1024,NPMAX
                 PRINT 1020
                 M1=M1+1
                 DO 65 JJ=1,NMAX
            65 PRINT 1021,NLIST(JJ)
            90  CONTINUE
           100 CONTINUE
           110 CONTINUE
                 STOP 88
                 END
```

```
002  COMPILE   RUN  AUTOCODER                                                  POGO
003  EXECUTE   CNTRL7                                                         FINDR
004            DC
005                 @FINDER    @
006                 +0+0+325+325+910C000001
007  ORIGIN    CNTRL325       SUBROUTINE FINDER(L,M,N,NK,NKV,NMAX,NLIST,
008  XRESERVE  CNTRL11-21                                  IBV,JBV,NP,K)
009            XZA  98,11
010            RS   98,SAVEIWS
011            BLX  94,0+X94
012            XU   94,RETURNIW
013            ZA1  +0          ZERO NLIST
014            XL   NX,0+X20
015            XZA  NX,1
016            XL   10,17
017  ZERON     ZST1 0+X10
018            XA   10,1
019            BIX  NX;ZERON
020            ZA1  0+X11
021            S1   +2
022            BZ1  STARTL2
023            BM1  STARTL1
024            B    STARTL3
030  STARTL1   ZS1  12(1,5)    FORM MRDW
031            ZST1 MRDW(1,5)
033            S1   0+X13
034            A1   +1
035            STD1 MRDW(6,9)
036            XL   NX,0+X13  FIND KS OCCURING LEAST OFTEN
037            XZA  NX,1
038            ZA1  +1
039            XL   10,12
040  ADDONE    ZA2  0(7,9)+X10  FORM LIST OF HOW MANY K1S,K2S,ETC.
041            S2   +1
042            STD2 *(7,9)+1
043            AS1  0+X17
044            XA   10,1
045            BIX  NX,ADDONE
046            ZA3  +9999999999  LOOK UP K OR KS FOUND LEAST NO.OF TIMES
047            XSN  98,1
048            ZS1  17(1,5)
049            SL1  4
050            S1   17(2,5)
051            S1   0+X20
052            A1   +1
053            ZST1 NLISTRDW
0531           XL   ZMX,ZMULTAREA
0532 LOOK      LL   NLISTRDW
0533           NOP
0534           BZ3  *+3
0535           ZST3 0+X15
0536           B    CONT
0537           ZA3  +99999
0538           ZST3 0+X98
0539           ZA1  98(1,5)
0540           A1   +1
0541           S1   17(1,5)
0542           ZST1 0+ZMX
0544           BIX  ZMX,LOOK
057  CONT      ZA1  98(1,5)
058            A1   +1
059            S1   17(1,5)
060            ZST1 NLISTRDW+1
```

```
061              XL    NX,+10000
062              ZA1   +9999999999
063  ANOTHERK    ZST1  0+X98      FORM LIST OF K VALUES
065              LE    NLISTRDW
066              B     NOMORE
067              ZA2   98(1,5)
068              A2    +1
069              S2    17(1,5)
070              ZST2  NLISTRDW+1+NX
071              BIX   NX,ANOTHERK
0711 NOMORE      ZA1   NX(2,5)
0712             ZST1  0+X14
0713             ZA1   ZMX(2,5)
0714             S1    ZMULTAREA(2,5)
0715             ZST1  0+X16
0716             BZ1   RETURN
0717             XS    ZMX,1
0718             XLIN  ZMX,ZMX
0719             ZA1   ZMULTAREA(2,5)
0720             STD1  ZMX(2,5)
0721             MSM   ZMX
0722             RG    17,ZMX
073              B     RETURN
080  STARTL2     XLIN  10,0+X14     SEARCH FOR ALL IOR J =K
0801             ZA3   NLISTRDW+X10
0805             ZST3  0+X21
081              XL    10,MRDW
082              XL    KX,+0
083              XL    NX,17
0835             ZA2   +99999
084              XSN   98,1
0845 ANOTHERI    LE    10(1,3)    FOR I=K STORE J IN LIST
085              B     NOMOREIK
0855             C2    0(4,6)+X98
0856             BE    *+6
086              ZA2   0(4,6)+X98
087              ZST2  0+NX
088              XA    NX,1
089              XZS   10,0+X98
090              XA    KX,1
091              BIX   10,ANOTHERI
092  NOMOREIK    XL    10,MRDW    FOR J=K STORE I IF NEW VALUE
094  ANOTHERJ    LE    10(4,6)
095              B     NOMOREJK
096              ZA3   0(1,3)+X98
097              XZS   10,0+X98
099              LE    NLISTRDW   IS I A NEW VALUE
100              B     YES
101              B     NO
102  YES         ZST3  0+NX
103              XA    NX,1
104              XA    KX,1
105  NO          ZA3   NLISTRDW+X14
106              BIX   10,ANOTHERJ
107  NOMOREJK    ZA1   KX(2,5)
108              ZST1  0+X16
109              ZA1   MRDW
110              ZST1  MRDWP
111              B     SORT
120  STARTL3     XLIN  10,0+X14
1201             ZA3   NLISTRDW+X10
121              XSN   98,1
122              LE    MRDWP(7,9)  FIND AN I AND J OF BASIS VECTOR OF K
```

```
1221             B     23456  ERROR
123              ZA1   98(1,5)       (PREPARE ROW FOR NEXT LE)
124              A1    +1
125              STD1  MRDWP(1,5)
126              ZA3   0(1,3)+X98
127              ZST3  0+X18            IBV
128              ZA1   0(4,6)+X98
129              ZST1  0+X19            JBV
130              XL    NX,17
131              XL    MX,MRDW    SEARCH M LIST FOR I VALUE AND LIST ITS
133  SEARCHI     LE    MX(1,3)          J IN NLIST(1,3)
134              B     NOMOREI
135              ZA1   0(4,6)+X98
136              ZST1  0(1,3)+NX
137              XA    NX,1
138              XZS   MX,0+X98
139              BIX   MX,SEARCHI
1391 NOMOREI     XL    MX,MRDW
1393 SEARCHI2    LE    MX(4,6)
1394             B     NOMOREI2
1395             ZA1   0(1,3)+X98
1396             ZST1  0(1,3)+NX
1397             XA    NX,1
1398             XZS   MX,0+X98
1399             BIX   MX,SEARCHI2
140  NOMOREI2    ZA3   0+X19      SEARCH M LIST FOR J VALUE AND LIST ITS I
141              XL    KX,17        IN NLIST(4,6)
142              XL    MX,MRDW
144  SEARCHJ     LE    MX(4,6)
145              B     NOMOREJ
146              ZA1   0(1,3)+X98
147              STD1  0(4,6)+KX
148              XA    KX,1
149              XZS   MX,0+X98
150              BIX   MX,SEARCHJ
1501 NOMOREJ     XL    MX,MRDW
1503 SEARCHJ2    LE    MX(1,3)
1504             B     NOMOREJ2
1505             ZA1   0(4,6)+X98
1506             STD1  0(4,6)+KX
1507             XA    KX,1
1508             XZS   MX,0+X98
1509             BIX   MX,SEARCHJ2
151  NOMOREJ2    XS    NX,1
1511             XLIN  NX,NX      PICK NOS COMMON TO I AND J LISTS
152              XZS   NX,0+X17
153              XU    NX,NLISTRDW
1531             XS    KX,1
154              XLIN  KX,KX
155              XZA   KX,0+X17
156              MSP   NX
157              ZA3   +99999
1572 LOOKAGN     C3    0(4,6)+KX
1573             BE    NOCOMMON
1574             ZA3   0(4,6)+KX
159              LE    NLISTRDW(1,3)
160              B     NOCOMMON
161              STD3  0(7,9)+NX    STORE COMMON NOS IN NLIST(7,9)
162              XA    NX,1
163  NOCOMMON    BIX   KX,LOOKAGN
1631             ZA1   NX(2,5)      HOW MANY IN NLIST-NMAX
1632             S1    17(2,5)
1633             ZST1  0+X16
```

```
164              ZA1   +0                ZERO REST OF LIST
165              XL    NX,NLISTRDW
166              MSP   NX
167  ZERO        ST1   0(0,6)+NX
168              BIX   NX,ZERO
1685 SORT        ZA1   0+X16
1686             A1    17(2,5)
1687             S1    +1
1688             XL    LISTX,99991
1689             XZA   LISTX,0+X17
1690 SORT3       MSM   LISTX
1691             ZA3   +999
1693             LL    LISTX
16935            B     23457  ERROR
1694             MSP   LISTX
1695             ZA1   0+LISTX
1696             ZST3  0+LISTX
1697             ZST1  0+X98
1698             BIX   LISTX,SORT3
173  RETURN      XZA   98,11
174              RG    98,SAVEIWS
175              XL    94,RETURNIW
176              B     0+X94
177  SAVEIWS     DRDW  -**1,**14
178              DA    1
179                    0,139
180  RETURNIW          140,149
181  MRDW              150,159
182  MRDWP             160,169
183  NLISTRDW          170,1669
1831 ZMULTAREA   DA    1,+RDW
1832                   0,1499
184  END         CNTRL325
185
```