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Mathematics
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MASTER

A BASIC LANGUAGE COMPUTER PROGRAM
FOR CALCULATING INTERPLANAR SPACINGS

P. R. Budelov

J. R. Cullipher

UNION CARBIDE CORPORATION
NUCLEAR DIVISION
OAK RIDGE Y-12 PLANT

operated for the ATOMIC ENERGY COMMISSION under U. S. GOVERNMENT Contract W-7405 eng 26

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ABSTRACT

A computer program has been developed for calculating the interplanar spacings (d , Å) of a crystal, given the crystal system and the lattice parameters. The program, written in the BASIC computer language, generates and prints only valid Miller indices and interplanar spacings for the crystal system specified.

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SUMMARY

A computer program has been developed for listing Miller indices and calculating interplanar spacings (d , A) of compounds from knowledge of the lattice parameters and crystal system. In many instances, listings of Miller indices and interplanar spacings are not readily available. This program can furnish such information if the crystal type and lattice parameters are known. The program, written in the BASIC computer language, generates and prints only valid Miller indices and interplanar spacings for the crystal system specified.

Incorporated in the program are the Bravais lattices, which are the crystal systems most often encountered in X-ray diffraction analyses. Also, provisions were made for several special cases which were encountered frequently in the literature.

INTRODUCTION

Lattice parameters and the crystal-system designations for compounds not listed in the powder diffraction file of the American Society for Testing Materials⁽¹⁾ are often available in other literature; however, in most cases, a listing of the Miller indices and interphase spacings are not readily available. The computer program described in this report avoids the laborious task of calculating this information by hand.

The program is intended for use with time-sharing computer systems that utilize BASIC as the language⁽²⁾. It is written to give the user with little or no previous training in computer programming a simple and straight-forward method of calculating interplanar spacing.

COMPUTER CALCULATION OF INTERPLANAR SPACINGS

PROGRAM DESCRIPTION

A series of 19 different programs is used. There is one fundamental program called INTPA. The other 18 subprograms each have a separate name which corresponds either to one of the Bravais lattices or to one of the special cases. General instructions, which include all of the program names, are given in Appendix A. Combining INTPA with any one of the 18 subprograms is accomplished by executing the EDIT WEAVE command. A printout is thus obtained of all valid Miller indices and their respective interplanar spacings for the desired crystal system. Also, a general restriction in INTPA excludes the printing of d less than 1.000 Å.

The programs, listed in Appendix A, are written in the BASIC computer language.⁽²⁾

The data input is Line 8000 of INTPA. New data are put in by retyping Line 8000 with the new values in accordance with the BASIC data format. The INTPA program computes all necessary variables for calculating the interplanar spacing, but it does not define values for the Miller indices. Each subprogram selects the correct values of H, K, and L for that particular crystal system. The EDIT WEAVE command is used to join INTPA with one of the subprograms. This command has the format:

EDIT WEAVE INTPA, NNNNN,

where NNNNN represents the name of any one of the 18 subprograms. This command will merely join INTPA and NNNNN together. Each of the 18 subprograms have line numbers that start at either 500 or 1000 and all end before 7000; thus, when weaved with INTPA, each subprogram will fit into INTPA between Lines 100 and 7000. The EDIT WEAVE command does not resequence the joined programs, it just fuses the two together.

It is necessary, however, that INTPA and NNNNN have both been saved prior to giving the EDIT WEAVE command.

Output is printed in four separate columns with the headings D, H, K, and L. Column D represents the interplanar distance in angstroms; Columns H, K, and L represent the Miller indices for the corresponding D column. Printed at the head of the column is the name of the particular crystal system being used, and printed at the bottom of the column are the lattice parameters used. In some of the programs there are some invalid H, K, L, and D values that are inevitably generated. In these cases, the invalid Miller indices are listed at the top of the sheet and identified with the title, "Values not Needed". Thus, the invalid values can be crossed off from the listing.

DISCUSSION

Calculation of the interplanar spacing in all of these programs is done in the fundamental program, INTPA. The triclinic equation that relates d to the lattice parameters (a , b , c , δ , β , and γ) and to the Miller indices is used as the basis of the computation.

This equation can be used for the triclinic and all the other crystal systems by placing all six lattice parameters of the desired system into the DATA statement. Since the triclinic system possesses the lowest symmetry and thereby requires the definition of all six parameters, it can be used as a general equation for all the other crystal systems. Restrictions are placed on the Miller indices considered for computation according to the extinction rules for each Bravais type of lattice.⁽³⁾ There were other restrictions that were simply observed by accumulating as many ASTM cards as practical for a certain kind of crystal and noting a similarity or relationship between all the valid indices.⁽¹⁾ All restrictions are included in a separate program for each system; they are used with INTPA when joined together by the EDIT WEAVE command.

In the RMHDL program for the rhombohedral system, the lattice parameters are converted to hexagonal parameters and then computed with Miller indices based on the hexagonal crystal system. Therefore, the listed Miller indices will refer to the hexagonal unit cell rather than the rhombohedral.

The last three lines of TRCLN, the triclinic program, appear to be a waste of storage space. If, however, these lines are omitted, an error statement ("next" without "for") will be encountered. Since INTPA must be joined with TRCLN to obtain answers and since INTPA must contain the three "next" statements due to the need for them in the other 17 programs, three dummy "for" statements must be included in the TRCLN program; hence, Lines 2880, 2890, and 2900 must be included.

There are several modifications that can be made on these programs. The most important modification is the extension of the limits of the Miller indices being generated. For some crystals, the lattice parameters may be so large that it would be desirable to generate Miller indices that are larger than those furnished in the program. This step is accomplished by retyping the "for" statements for the Miller indices. For example, in the simple cubic, the limits are 15, 15, 15 for H, K, and L. To extend H to 20, K to 25, and L to 30, call old program SMCUB and type:

```
550 FOR L = 0 to 30,
560 FOR K = 0 to 25, and
570 FOR H = 0 to 20.
```

Then, the computer must be instructed to command SAVE to retain the changes as part of the program. For the simple cubic, the line numbers are 550, 560, and 570.

In some programs they are 1050, 1060, and 1070, but these line numbers are easy enough to determine by inspection of the program listing.

If all of the valid interplanar spacings were allowed to be printed when the limits on H, K, and L were as high as 10, 20, or 30, then many unwanted values would be printed also. To avoid this, a restriction is applied in Statement 7030 of INTPA which will restrict any values of d less than 1.000 from being printed. If a lower or higher cutoff value is desired, simply call old program INTPA and retype Line 7030 as follows:

7030 If $D < X.XXX$ then 7050,

where X.XXX represents the desired cutoff value and 7050 will send the computer on to calculate the next value.

The advantage of maintaining large limits on the indices and a reasonable cutoff point on d is that a small correct list will be printed for a crystal with small parameters, and a large valid list will be printed for a crystal with large parameters.

When the results of the programs are compared with the ASTM data for the same compound, discrepancies may seem evident. First, the d values from the program and those on an ASTM card may not correspond exactly, and certain Miller indices generated by the program may not show up on a diffraction pattern for the same compound. The reasons here are that the d values on ASTM cards are often observed values with inherent measurement errors. The resulting computation of values for d from the computer are theoretical values computed from the lattice parameters. The reason for the second discrepancy is that the intensity of some of the reflections will be too low to show up, although they are still valid.

The interplanar spacings and Miller indices generated by these programs have been compared with ASTM X-ray diffraction powder data file.⁽³⁾ Lattice parameters for compounds of each crystal system were taken from the file and the resulting values of d and Miller indices were compared with those listed in the file for the appropriate compound. An example of the computer listings obtained for a typical compound, thallium fluoride, is compared with ASTM data in Appendix B.

CONCLUSIONS

This report was intended to give the user with little or no previous training in computer programming a simple and straight-forward method of calculating interplanar spacings. FORTRAN, which most industrial computers use, is a more mathematically oriented language than the BASIC language used in these programs and is thus more difficult. With a time-sharing system, the user can type in, run the program, and get the answers all within a reasonable amount of time.

The programs presented here are useful in calculating the interplanar spacings of compounds not listed in the ASTM powder data file when the lattice parameters of the compounds are available. In the cases where the ASTM file does not list the Miller indices, the programs can furnish such information if the crystal type and lattice parameters are known.

The general equation for calculating d is contained in the fundamental program, INTPA. The purpose of each of the eighteen subprograms is to impose the correct restrictions on the Miller indices for each specific crystal form.

As stated previously, the generating limits of the Miller indices can be altered to suit the user's desires. Larger limits will give a more complete list, but the possibility of very low intensities or invalid values may increase at the same time.

REFERENCES

- (1) X-Ray Powder Data File, American Society for Testing Materials, Philadelphia, Pennsylvania.
- (2) Kemeny, John G. and Kurtz, Thomas E.; A Manual for BASIC, C-E-I-R, Inc (1965).
- (3) Klug, Harold P. and Alexander, LeRoy, E.; X-Ray Diffraction Procedures for Polycrystalline and Amorphous Materials; John Wiley and Sons, Inc, New York, New York (1954).

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APPENDIX A

GENERAL INSTRUCTIONS

```

1  SAVED BY J. E. FERGUSON 10/27/67 PH.35944, Y-12
2
3
4  INTPA*, WHEN COMBINED WITH ONE OF THE FOLLOWING SUB-PROGRAMS,
5  COMPUTES AND PRINTS VALID INTER-PLANAR DISTANCES AND MILLER
6  INDICES FOR A CRYSTAL, GIVEN THE SYSTEM, LATTICE PARAMETERS,
7  AND INTERAXIAL ANGLES.
8
9  ANY ONE OF 18 DIFFERENT CRYSTAL TYPES CAN BE USED.
10 THE SUB-PROGRAMS ARE:
11
12
13  SMCUB* - SIMPLE CUBIC
14  BDCUB* - BODY CENTERED CUBIC
15  FCCUB* - FACE CENTERED CUBIC
16  SMTET* - SIMPLE TETRAGONAL
17  BDTET* - BODY CENTERED TETRAGONAL
18  FCTET* - FACE CENTERED TETRAGONAL
19  SMORT* - SIMPLE ORTHORHOMBIC
20  BDORT* - BODY CENTERED ORTHORHOMBIC
21  BSOTA* - BASE CENTERED ORTHORHOMBIC ON THE A AXIS
22  BSOTB* - BASE CENTERED ORTHORHOMBIC ON THE B AXIS
23  BSOTC* - BASE CENTERED ORTHORHOMBIC ON THE C AXIS
24  FCORT* - FACE CENTERED ORTHORHOMBIC
25  HEXAG* - HEXAGONAL
26  RMHDL* - RHOMBOHEDRAL
27  RMHEX* - RHOMBOHEDRAL INDEXED ON HEXAGONAL AXES
28  SMMON* - SIMPLE MONOCLINIC
29  BSMON* - BASE CENTERED MONOCLINIC
30  TRCLN* - TRICLINIC
31
32
33  TO USE, PLACE THE DESIRED SUB-PROGRAM NNNNN* IN LOCAL
34  STORAGE BY RENAMING NNNNN (OMIT ASTERISK) AND SAVE.
35
36  RENAME INTPA* INTPA AND SAVE.
37
38
39  COMMAND:
40      EDIT WEAVE INTPA,NNNNN
41
42
43  INSERT DATA STATEMENT:
44      8000 DATA AA.AA,BB.BB,CC.CC,XX.XX,YY.YY,ZZ.ZZ
45
46  WHERE AA.AA,BB.BB,CC.CC ARE THE CRYSTAL LATTICE DIMENSIONS AND
47  XX.XX,YY.YY,ZZ.ZZ ARE THE AXIAL ANGLES. ALL 6 DATA MUST BE
48  INCLUDED.
49
50
51  COMMAND:
52      RUN

```

COMPUTER PROGRAMS

```

INTPA      16:03   CEIR   08/15/67

25 REM SAVED BY J.R.CULLIPHER ON 6/30/67, PH. 3-5944, Y-12
30 REM TO COMPUTE THE DISTANCE BETWEEN ADJACENT PLANES OF A
35 REM CRYSTAL GIVEN CRYSTAL SYSTEM AND LATTICE PARAMETERS.
40 READ A, B, C, A7, B7, C7
45 LET A1 = A7*6.28318/360.
50 LET A2 = B7*6.28318/360.
55 LET A3 = C7*6.28318/360.
60 LET Z = 2*COS(A1)*COS(A2)*COS(A3)
65 LET Y = -1*(COS(A1))^2-(COS(A2))^2-(COS(A3))^2
70 LET V = A*B*C*SQR(1+Y+Z)
75 LET A8=(B^2)*(C^2)*(SIN(A1))^2
80 LET B8=(A^2)*(C^2)*(SIN(A2))^2
85 LET C8=(A^2)*(B^2)*(SIN(A3))^2
90 LET D8=A*B*(C^2)*(COS(A1)*COS(A2)-COS(A3))
95 LET E8=(A^2)*B*C*(COS(A2)*COS(A3)-COS(A1))
100 LET F8=A*(B^2)*C*(COS(A3)*COS(A1)-COS(A2))
1000 LET W = A8 * (H^2)+B8*(K^2) + C8* (L^2)
1010 LET V8 = 2*D8*H*K + (2*E8*K*L) + 2*F8*H*L
1020 LET D = SQR((V^2) / (W+V8))
1030 IF D<1.0 THEN 7050
1040 PRINT D, H;K;L
1050 NEXT H
1060 NEXT K
1070 NEXT L
1080 PRINT
1090 PRINT
1100 PRINT"THE LATTICE PARAMETERS ARE:  A=" A, "B=" B, "C=" C
1110 PRINT"                                ALPHA="A7, "BETA="B7, "GAMMA="C
1120 PRINT
8000 DATA
9999 END

```

Figure A-1. INTPA - FUNDAMENTAL PROGRAM.

```

SMCUB      16:03   CEIR   08/15/67

500 REM SAVED BY J.R. CULLIPHER ON 6/30/67. PH.3-5944, Y-12
510 PRINT"          SIMPLE CUBIC"
520 PRINT
530 PRINT
540 PRINT "      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 15
560 FOR K = 0 TO 15
570 FOR H = 0 TO 15
580 IF H+K+L = 0 THEN 7050
590 IF H<K THEN 7050
600 IF K<L THEN 7050

```

Figure A-2. SMCUB - SIMPLE CUBIC.

```

BDCUB      16:22   CEIR   08/15/67

500 REM  SAVED BY J.R. CULLIPHER ON 6/30/67, PH.35044, Y-12
510 PRINT"          BODY CENTERED CUBIC"
520 PRINT
530 PRINT
540 PRINT "      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 15
560 FOR K = 0 TO 15
570 FOR H = 0 TO 15
580 IF H+K+L = 0 THEN 7050
590 LET E = 2
600 LET N = H+K+L
610 IF N-E > 0 THEN 640
620 IF N-E < 0 THEN 7050
630 IF N-E = 0 THEN 660
640 LET E = E+2
650 GOTO 610
660 IF H<K THEN 7050
670 IF K<L THEN 7050

```

Figure A-3. BDCUB - BODY CENTERED CUBIC.

```

FCCUB      16:13   CEIR   08/15/67

500 REM  SAVED BY J.R. CULLIPHER ON 6/30/67 PH.3-5944, Y-12
510 PRINT"          FACE CENTERED CUBIC"
520 PRINT
530 PRINT
540 PRINT "      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 15
560 FOR K = 0 TO 15
570 FOR H = 0 TO 15
580 IF H+K+L = 0 THEN 7050
590 IF K+L = 0 THEN 670
600 LET E = 2
610 LET N = K+L
620 IF N-E > 0 THEN 650
630 IF N-E < 0 THEN 7050
640 IF N-E = 0 THEN 670
650 LET E = E + 2
660 GO TO 620
670 LET E = 2
680 LET N = H+K
690 IF N-E > 0 THEN 720
700 IF N-E < 0 THEN 7050
710 IF N-E = 0 THEN 740
720 LET E = E + 2
730 GO TO 690
740 IF H<K THEN 7050
750 IF K<L THEN 7050

```

Figure A-4. FCCUB - FACE CENTERED CUBIC.

```

SMTET      9:30   CEIR   08/16/67

1000 REM  SAVED BY J.R. CULLIPHER ON 6/30/67 PH.3-5944, Y-12
1010 PRINT"          SIMPLE TETRAGONAL"
1020 PRINT
1030 PRINT
1040 PRINT "      D", " H"; "      K"; "      L"
1050 FOR L=0 TO 10
1060 FOR K=0 TO 10
1070 FOR H=0 TO 10
1080 IF H+K+L = 0 THEN 7050
1090 IF H<K THEN 7050
1100 IF K=4 THEN 1120
1110 GOTO 1130
1120 IF H = 5 THEN 7050
1130 IF L = 3 THEN 1150
1140 GOTO 1340
1150 IF K = 0 THEN 1170
1160 GOTO 1190
1170 IF H<5 THEN 7000
1180 GOTO 7050
1190 IF K=1 THEN 1170
1200 GOTO 1210
1210 IF K = 2 THEN 1230
1220 GOTO 1250
1230 IF H<4 THEN 7000
1240 GOTO 7050
1250 IF K = 3 THEN 1270
1260 GOTO 1300
1270 IF H=4 THEN 7050
1280 IF H<6 THEN 7000
1290 GOTO 7050
1300 IF K = 4 THEN 1320
1310 GOTO 7050
1320 IF H=6 THEN 7000
1330 GOTO 7050
1340 IF L = 4 THEN 1360
1350 GOTO 1510
1360 IF K = 0 THEN 1380
1370 GOTO 1400
1380 IF H>4 THEN 7050
1390 GOTO 7000
1400 IF K = 1 THEN 1420
1410 GOTO 1440
1420 IF H>3 THEN 7050
1430 GOTO 7000
1440 IF K=3 THEN 7050
1450 IF K = 2 THEN 1470
1460 GOTO 7050
1470 IF H=4 THEN 7050
1480 IF H>6 THEN 7050
1490 IF H=5 THEN 7050
1500 GOTO 7000
1510 IF L = 0 THEN 1530
1520 GOTO 1700
1530 IF K=0 THEN 7000
1540 IF K=1 THEN 1560
1550 GOTO 1580
1560 IF H>5 THEN 7050

1570 GOTO 7000
1580 IF K=2 THEN 7000
1590 IF K = 3 THEN 1610
1600 GOTO 1650
1610 IF H=6 THEN 7000
1620 IF H=3 THEN 7000
1630 IF H=5 THEN 7000
1640 GOTO 7050
1650 IF K=4 THEN 1670
1660 GOTO 7050
1670 IF H=4 THEN 7000
1680 IF H=6 THEN 7000
1690 GOTO 7050
1700 IF L=1 THEN 1720
1710 GOTO 1860
1720 IF K = 0 THEN 1740
1730 GOTO 1760
1740 IF H>5 THEN 7050
1750 GOTO 7000
1760 IF K=1 THEN 7000
1770 IF K = 2 THEN 1790
1780 GOTO 1810
1790 IF H<8 THEN 7000
1800 GOTO 7050
1810 IF K = 3 THEN 1790
1820 IF K=4 THEN 1840
1830 GOTO 7050
1840 IF H=4 THEN 7000
1850 GOTO 7050
1860 IF L= 2 THEN 1880
1870 GOTO 2070
1880 IF K = 0 THEN 1900
1890 GOTO 1920
1900 IF H<7 THEN 7000
1910 GOTO 7050
1920 IF K = 1 THEN 1940
1930 GOTO 1970
1940 IF H=6 THEN 7050
1950 IF H>7 THEN 7050
1960 GOTO 7000
1970 IF K = 2 THEN 1990
1980 GOTO 2010
1990 IF H<7 THEN 7000
2000 GOTO 7050
2010 IF K=3 THEN 2030
2020 GOTO 2050
2030 IF H>5 THEN 7050
2040 GOTO 7000
2050 IF K = 4 THEN 1990
2060 GOTO 7050
2070 IF L = 5 THEN 2090
2080 GOTO 2220
2090 IF K = 0 THEN 2110
2100 GOTO 2140
2110 IF H=4 THEN 7050
2120 IF H>5 THEN 7050
2130 GOTO 7000
2140 IF K=1 THEN 2160
2150 GOTO 2180
2160 IF L<4 THEN 7000

2170 GOTO 7050
2180 IF K=2 THEN 2200
2190 GOTO 7050
2200 IF H>4 THEN 7050
2210 GOTO 7000
2220 IF L = 6 THEN 2240
2230 GOTO 2410
2240 IF K= 0 THEN 2260
2250 GOTO 2290
2260 IF H< 3 THEN 7000
2270 IF H=6 THEN 7000
2280 GOTO 7050
2290 IF K = 1 THEN 2310
2300 GOTO 2330
2310 IF H<4 THEN 7000
2320 GOTO 7050
2330 IF K=2 THEN 2350
2340 GOTO 2370
2350 IF H= 4 THEN 7000
2360 GOTO 7050
2370 IF K = 4 THEN 2390
2380 GOTO 7050
2390 IF H=6 THEN 7000
2400 GOTO 7050
2410 IF L= 7 THEN 2430
2420 GOTO 2480
2430 IF K=0 THEN 2450
2440 GOTO 7050
2450 IF H=0 THEN 7050
2460 IF H<3 THEN 7000
2470 GOTO 7050
2480 IF L = 8 THEN 2500
2490 GO TO 7000
2500 IF K = 0 THEN 2520
2510 GOTO 2560
2520 IF H=0 THEN 7000
2530 IF H=4 THEN 7000
2540 IF H=1 THEN 7000
2550 GOTO 7050
2560 IF K=1 THEN 2580
2570 GOTO 2600
2580 IF H=1 THEN 7000
2590 GOTO 7050
2600 IF K = 2 THEN 2620
2610 GOTO 7050
2620 IF H=2 THEN 7000
2630 GOTO 7050

```

Figure A-5. SMTET - SIMPLE TETRAGONAL.

```

BDTET      9:40   CEIR   08/16/67

500 REM SAVED BY J.R. CULLIPHER ON 6/30/67, PH.35944, Y-12
505 PRINT"          BODY CENTERED TETRAGONAL"
510 PRINT
515 PRINT
520 PRINT"      D", " H"; "      K"; "      L"
525 FOR L = 0 TO 6
530 FOR K = 0 TO 5
535 FOR H = 0 TO 6
540 IF H+K+L = 0 THEN 7050
545 LET E = 2
550 LET N = H+K+L
555 IF N-E > 0 THEN 570
560 IF N-E < 0 THEN 7050
565 IF N-E = 0 THEN 580
570 LET E = E+2
575 GOTO 555
580 IF H<K THEN 7050
585 IF L=1 THEN 595
590 GOTO 715
595 IF (H+2) + (K+2) = 5 THEN 7000
600 IF (H+2) + (K+2) = 13 THEN 7000
605 IF K=4 THEN 7000
610 IF K= 0 THEN 620
615 GOTO 635
620 IF H=3 THEN 7000
625 IF H=1 THEN 7000
630 GO TO 7050
635 IF K = 2 THEN 645
640 GOTO 655
645 IF H=5 THEN 7000
650 GO TO 7050
655 IF K = 3 THEN 665
660 GOTO 675
665 IF H= 6 THEN 7000
670 GO TO 7050
675 IF K= 5 THEN 685
680 GOTO 695
685 IF H = 6 THEN 7000
690 GO TO 7050
695 IF K = 1 THEN 705
700 GOTO 715
705 IF H = 4 THEN 7000

```

```

710 GO TO 7050
715 IF L = 3 THEN 725
720 GOTO 830
725 IF K = 0 THEN 735
730 GOTO 755
735 IF H = 1 THEN 7000
740 IF H= 3 THEN 7000
745 IF H = 5 THEN 7000
750 GO TO 7050
755 IF K = 1 THEN 765
760 GOTO 785
765 IF H = 1 THEN 7000
770 IF H= 2 THEN 7000
775 IF H = 4 THEN 7000
780 GO TO 7050
785 IF K = 2 THEN 795
790 GOTO 810
795 IF H = 3 THEN 7000
800 IF H = 5 THEN 7000
805 GO TO 7050
810 IF K = 3 THEN 820
815 GO TO 7050
820 IF H = 4 THEN 7000
825 GO TO 7050
830 IF L = 5 THEN 840
835 GO TO 7000
840 IF K = 0 THEN 850
845 GOTO 865
850 IF H = 1 THEN 7000
855 IF H = 3 THEN 7000
860 GO TO 7050
865 IF K = 1 THEN 875
870 GO TO 7050
875 IF H = 1 THEN 7000
880 IF H = 2 THEN 7000
885 IF H = 4 THEN 7000
890 GO TO 7050

```

Figure A-6. BDTET - BODY CENTERED TETRAGONAL.

```

FCTET      9:45   CEIR   08/16/67

500 REM SAVED BY J.R. CULLIPHER ON 6/23/67, PH.35944, Y-12
510 PRINT"          FACE CENTERED TETRAGONAL"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+L = 0 THEN 7050
590 IF H=0 THEN 610
600 GOTO 690
610 IF K = 0 THEN 630
620 GOTO 690
630 LET E = 2
640 IF L-E > 0 THEN 670
650 IF L-E < 0 THEN 7050
660 IF L-E = 0 THEN 7000
670 LET E = E + 2
680 GOTO 640
690 IF L=0 THEN 710
700 GOTO 790
710 IF K=0 THEN 730
720 GOTO 790
730 LET E = 2
740 IF H-E > 0 THEN 770
750 IF H-E < 0 THEN 7050
760 IF H-E = 0 THEN 7000
770 LET E = E+2
780 GOTO 740
790 IF H<K THEN 7050
800 LET E = 2
810 LET N = H+K
820 IF N-E > 0 THEN 850
830 IF N-E < 0 THEN 7050
840 IF N-E = 0 THEN 870
850 LET E = E+2
860 GOTO 820
870 LET E = 2
880 LET N = H+L
890 IF N-E > 0 THEN 920
900 IF N-E < 0 THEN 7050
910 IF N-E = 0 THEN 940
920 LET E = E+2
930 GOTO 890
940 LET E = 2
950 LET N = K+L
960 IF N-E > 0 THEN 990
970 IF N-E < 0 THEN 7050
980 IF N-E = 0 THEN 7000
990 LET E = E+2
999 GO TO 960

```

Figure A-7. FCTET - FACE CENTERED TETRAGONAL.

```

SMORT      9:52   CEIR   08/16/67
500 REM SAVED BY J.R.CULLIPHER ON 6/30/67, PH.3-5944, Y-12
505 PRINT"          SIMPLE ORTHORHOMBIC"
510 PRINT
515 PRINT
520 PRINT"      D", " H"; "      K"; "      L"
525 FOR L = 0 TO 10
530 FOR K = 0 TO 10
535 FOR H = 0 TO 10
540 IF H+K+L = 0 THEN 7050
545 IF L=0 THEN 555
550 GOTO 630
555 IF K=0 THEN 565
560 GOTO 575
565 IF H=5 THEN 7050
570 GOTO 7000
575 IF K=1 THEN 585
580 GOTO 595
585 IF H=0 THEN 7050
590 GOTO 7000
595 IF K=3 THEN 585
600 IF K=5 THEN 585
605 IF K=4 THEN 615
610 GOTO 625
615 IF H=6 THEN 7050
620 GOTO 7000
625 IF K=6 THEN 565
630 IF L=1 THEN 640
635 GOTO 690
640 IF K=4 THEN 615
645 IF K=5 THEN 655
650 GOTO 670
655 IF H=5 THEN 7050
660 IF H=6 THEN 7050
665 GOTO 7000
670 IF K=6 THEN 680
675 GOTO 7000
680 IF H>2 THEN 7050
685 GOTO 7000
690 IF L=2 THEN 700
695 GOTO 765
700 IF K=3 THEN 710
705 GOTO 720

```

Figure A-8. SMORT - SIMPLE ORTHORHOMBIC.

```

710 IF H>3 THEN 7050
715 GOTO 7000
720 IF K=4 THEN 710
725 IF K=5 THEN 735
730 GOTO 745
735 IF H>2 THEN 7050
740 GOTO 7000
745 IF K=6 THEN 755
750 GOTO 7000
755 IF H>1 THEN 7050
760 GOTO 7000
765 IF L=3 THEN 775
770 GOTO 7000
775 IF K=0 THEN 785
780 GOTO 795
785 IF H=6 THEN 7050
790 GOTO 7000
795 IF K=1 THEN 785
800 IF K=2 THEN 810
805 GOTO 820
810 IF H>4 THEN 7050
815 GOTO 7000
820 IF K=3 THEN 830
825 GOTO 7000
830 IF H=3 THEN 7050

```

```

BDORT      9:59   CEIR   08/16/67
500 REM SAVED BY J.R.CULLIPHER ON 6/30/67, PH.35944, Y-12
510 PRINT"          BODY CENTERED ORTHORHOMBIC"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+L = 0 THEN 7050
590 LET E = 2
600 LET N = H+K+L
610 IF N-E > 0 THEN 640
620 IF N-E < 0 THEN 7050
630 IF N-E = 0 THEN 7000
640 LET E = E+2
650 GOTO 610

```

Figure A-9. BDORT - BODY CENTERED ORTHORHOMBIC.

```

BSOTA      10:00   CEIR   08/16/67
500 REM SAVED BY J.R.CULLIPHER ON 6/30/67 PH.3-5944, Y-12
510 PRINT"          BASE CENTERED ORTHORHOMBIC"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+L = 0 THEN 7050
590 IF L=0 THEN 610
600 GOTO 690
610 IF K=0 THEN 630
620 GOTO 690
630 LET E = 2
640 IF H-E > 0 THEN 670
650 IF H-E < 0 THEN 7050
660 IF H-E = 0 THEN 7000
670 LET E = E+2
680 GOTO 640
690 LET E = 2
700 LET N = K+L
710 IF N-E > 0 THEN 740
720 IF N-E < 0 THEN 7050
730 IF N-E = 0 THEN 7000
740 LET E = E+2
750 GOTO 710

```

Figure A-10. BSOTA - BASE CENTERED ORTHORHOMBIC ON THE A-AXIS.

```

BSOTB 10:01 CEIR 08/16/67
500 REM SAVED BY J.R.CULLIPHER ON 6/30/67 PH.3-5944, Y-12
510 PRINT"          BASE CENTERED ORTHORHOMBIC"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+L = 0 THEN 7050
590 IF L=0 THEN 610
600 GOTO 690
610 IF H=0 THEN 630
620 GOTO 690
630 LET E = 2
640 IF K-E >0 THEN 670
650 IF K-E <0 THEN 7050
660 IF K-E =0 THEN 7000
670 LET E = E+2
680 GOTO 640
690 LET E = 2
700 LET N = H+L
710 IF N-E >0 THEN 740
720 IF N-E <0 THEN 7050
730 IF N-E=0 THEN 7000
740 LET E = E+2
750 GOTO 710

```

Figure A-11. BSOTB - BASE CENTERED ORTHORHOMBIC ON THE B-AXIS.

```

BSOTC 10:03 CEIR 08/16/67
500 REM SAVED BY J.R.CULLIPHER ON 6/30/67 PH.3-5944, Y-12
510 PRINT"          BASE CENTERED ORTHORHOMBIC"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+L = 0 THEN 7050
590 IF K=0 THEN 610
600 GOTO 690
610 IF H=0 THEN 630
620 GOTO 690
630 LET E = 2
640 IF L-E >0 THEN 670
650 IF L-E <0 THEN 7050
660 IF L-E =0 THEN 7000
670 LET E = E+2
680 GOTO 640
690 LET E = 2
700 LET N = H+K
710 IF N-E >0 THEN 740
720 IF N-E <0 THEN 7050
730 IF N-E=0 THEN 7000
740 LET E = E+2
750 GOTO 710

```

Figure A-12. BSOTC - BASE CENTERED ORTHORHOMBIC ON THE C-AXIS.

```

FCORT 10:08 CEIR 08/16/67
500 REM SAVED BY J. R.CULLIPHER ON 6/26/67, PH.35944, Y-12
505 PRINT"          FACE CENTERED ORTHORHOMBIC"
510 PRINT
515 PRINT
520 PRINT"      D", " H"; "      K"; "      L"
525 FOR L = 0 TO 10
530 FOR K = 0 TO 10
535 FOR H = 0 TO 10
540 IF H+K+L = 0 THEN 7050
545 IF H=0 THEN 555
550 GOTO 595
555 IF K =0 THEN 565
560 GOTO 595
565 LET E = 2
570 IF L-E >0 THEN 585
575 IF L-E <0 THEN 7050
580 IF L-E =0 THEN 7000
585 LET E = E +2
590 GOTO 570
595 IF L=0 THEN 605
600 GOTO 645
605 IF K=0 THEN 615
610 GOTO 645
615 LET E = 2
620 IF H-E >0 THEN 635
625 IF H-E <0 THEN 7050
630 IF H-E =0 THEN 7000
635 LET E = E+2
640 GOTO 620
645 IF H+K =0 THEN 685
650 LET E = 2
655 LET N = H+K
660 IF N-E >0 THEN 675
665 IF N-E <0 THEN 7050
670 IF N-E = 0 THEN 685
675 LET E = E+2
680 GOTO 660
685 IF H+L =0 THEN 725
690 LET E =2
695 LET N= H+L
700 IF N-E >0 THEN 715
705 IF N-E <0 THEN 7050
710 IF N-E =0 THEN 725
715 LET E = E+2
720 GOTO 700
725 IF K+L =0 THEN 7000
730 LET E = 2
735 LET N = K+L
740 IF N-E >0 THEN 755
745 IF N-E <0 THEN 7050
750 IF N-E=0 THEN 7000
755 LET E = E+2
760 GOTO 740

```

Figure A-13. FCORT - FACE CENTERED ORTHORHOMBIC.

```

HEXAG      10:19   CEIR   09/22/67
500 REM   SAVED BY J.R.CULLIPHER ON 6/30/67 PH.35944, Y-12
510 PRINT"          HEXAGONAL"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = 0 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+L = 0 THEN 7050
590 IF H<K THEN 7050

```

Figure A-14. HEXAG - HEXAGONAL.

```

RMHDL      10:12   CEIR   08/16/67
500 REM   SAVED BY J.R.CULLIPHER ON 6/12/67 PH.35944, Y-12
505 LET A7 = A7*6.28318/360
510 LET A5 = A*2 * SIN (A7/2)
515 LET C5 = SQR(9*(A+2) - 3*(A5+2))
520 LET A = A5
525 LET B = A5
530 LET C = C5
535 LET A7 = 90
540 LET B7 = 90
545 LET C7 = 120
550 LET A1 = A7*6.28318/360
555 LET A2 = B7*6.28318/360
560 LET A3 = C7*6.28318/360
565 LET Z = 2*COS(A1)*COS(A2)*COS(A3)
570 LET Y = -1*(COS(A1))+2 - (COS(A2))+2 - (COS(A3))+2
575 LET V = A*B*C*SQR(1+Y+Z)
580 LET A8 = (B+2)*(C+2)*(SIN(A1))+2
585 LET B8 = (A+2)*(C+2)*(SIN(A2))+2
590 LET C8 = (A+2)*(B+2)*(SIN(A3))+2
595 LET D8 = A*B*(C+2)*(COS(A1)*COS(A2)-COS(A3))
600 LET E8 = (A+2)*B*C*(COS(A2)*COS(A3)-COS(A1))
605 LET F8 = A*(B+2)*C*(COS(A3)*COS(A1)-COS(A2))
610 PRINT"          RHOMBOHEDRAL"
615 PRINT
620 PRINT"VALUES NOT NEEDED ARE: 100, 500, 210, 320, 430, 001"
625 PRINT"111, 221, 421, 331, 531, 441, 551, 302, 502, 412, 522"
630 PRINT"203, 403, 313, 513, 423, 533, 553, 304, 504, 414, 524"
635 PRINT"544, 005, 505, 115, 225"
640 PRINT
645 PRINT"      D", " H"; "      K"; "      L"
650 FOR L = 0 TO 10
655 FOR K = 0 TO 10
660 FOR H = 0 TO 10
665 IF H+K+L = 0 THEN 7050
670 IF H<K THEN 7050
675 IF L=0 THEN 685
680 GOTO 695
685 IF K>3 THEN 7050
690 GOTO 910
695 IFL=5 THEN 705
700 GOTO 715
705 IF K>2 THEN 7050
710 GOTO 775
715 IF L=4 THEN 725
720 GOTO 775
725 IF K=0 THEN 745
730 IF K=1 THEN 755
735 IF K=2 THEN 765
740 GOTO 910
745 IF H=2 THEN 7000
750 GOTO 910
755 IF H=3 THEN 7000
760 GOTO 910
765 IF H=4 THEN 7000
770 GOTO 910
775 IF L=5 THEN 785
780 GOTO 835
785 IF K=0 THEN 805
790 IF K= 1 THEN 815
795 IF K= 2 THEN 825
800 GOTO 910
805 IF H=1 THEN 7000
810 GOTO 910
815 IF H=2 THEN 7000
820 GOTO 910
825 IF H= 3 THEN 7000
830 GOTO 910
835 IF L= 2 THEN 845
840 GOTO 880
845 IF K=0 THEN 860
850 IF K= 1 THEN 870
855 GOTO 910
860 IF H= 4 THEN 7000
865 GOTO 910
870 IF H=5 THEN 7000
875 GOTO 910
880 IF L=1 THEN 890
885 GOTO 910
890 IF K=0 THEN 900
895 GOTO 910
900 IF H=5 THEN 7000
905 GOTO 910
910 LET E = 2
915 IF H=K+L THEN 7000
920 LET N = H-K+L
925 IF N-E >0 THEN 940
930 IF N-E <0 THEN 7000
935 IF N-E =0 THEN 7050
940 LET E = E+2
945 GOTO 925

```

Figure A-15. RMHDL - RHOMBOHEDRAL.

RMHEX 10:18 CEIR 08/16/67

```

500 REM SAVED BY J.R.CULLIPHER ON 6/12/67, PH.35944, Y-12
505 PRINT " RHOMBOHEDRAL INDEXED ON HEXAGONAL AXES"
510 PRINT
515 PRINT "VALUES NOT NEEDED ARE: 100, 500, 210, 320, 430, 001"
520 PRINT "111, 221, 421, 331, 531, 441, 551, 302, 502, 412, 522"
525 PRINT "203, 403, 313, 513, 423, 533, 553, 304, 504, 414, 524"
530 PRINT "544, 005, 505, 115, 225"
535 PRINT
540 PRINT " D", " H"; " K"; " L"
545 FOR L = 0 TO 10
550 FOR K = 0 TO 10
555 FOR H = 0 TO 10
560 IF H+K+L = 0 THEN 7050
565 IF H<K THEN 7050
570 IF L=0 THEN 580
575 GOTO 590
580 IF K>3 THEN 7050
585 GOTO 805
590 IF L=5 THEN 600
595 GOTO 610
600 IF K>2 THEN 7050
605 GOTO 670
610 IF L=4 THEN 620
615 GOTO 670
620 IF K=0 THEN 640
625 IF K=1 THEN 650
630 IF K=2 THEN 660
635 GOTO 805
640 IF H=2 THEN 7000
645 GOTO 805
650 IF H=3 THEN 7000
655 GOTO 805
660 IF H=4 THEN 7000
665 GOTO 805
670 IF L=5 THEN 680
675 GOTO 730
680 IF K=0 THEN 700
685 IF K= 1 THEN 710
690 IF K= 2 THEN 720
695 GOTO 805
700 IF H=1 THEN 7000
705 GOTO 805

```

```

710 IF H=2 THEN 7000
715 GOTO 805
720 IF H=3 THEN 7000
725 GOTO 805
730 IF L= 2 THEN 740
735 GOTO 775
740 IF K=0 THEN 755
745 IF K= 1 THEN 765
750 GOTO 805
755 IF H=4 THEN 7000
760 GOTO 805
765 IF H=5 THEN 7000
770 GOTO 805
775 IF L=1 THEN 785
780 GOTO 805
785 IF K=0 THEN 795
790 GOTO 805
795 IF H= 5 THEN 7000
800 GOTO 805
805 LET E = 2
810 IF H= K+L THEN 7000
815 LET N = H-K+L
820 IF N-E >0 THEN 835
825 IF N-E <0 THEN 7000
830 IF N-E =0 THEN 7050
835 LET E = E+2
840 GOTO 820

```

Figure A-16. RMHEX - RHOMBOHEDRAL INDEXED ON HEXAGONAL AXIS.


```

SMMON      10:21      CEIR      08/16/67
500 REM   SAVED BY J.R.CULLIPHER ON 6/30/67, PH.3-5944, Y-12
510 PRINT"      SIMPLE MONOCLINIC"
520 PRINT
530 PRINT
540 PRINT"      D", " H"; "      K"; "      L"
550 FOR L = -10 TO 10
560 FOR K = 0 TO 10
570 FOR H = 0 TO 10
580 IF H+K+ ABS(L) =0 THEN 7050
590 IF H=0 THEN 610
600 GO TO 7000
610 IF L<0 THEN 7050
620 GO TO 7000

```

Figure A-17. SMMON - SIMPLE MONOCLINIC.

```

BSMON      10:29      CEIR      08/16/67
500 REM   SAVED BY J.R.CULLIPHER ON 6/29/67 PH.3-5944, Y-12
505 PRINT "      BASE CENTERED MONOCLINIC"
510 PRINT
515 PRINT
520 PRINT"      D", " H"; "      K"; "      L"
525 FOR L = 0 TO 10
530 FOR K = 0 TO 10
535 FOR H = -10 TO 10
540 IF ABS(H)+K+L =0 THEN 7050
545 IF L=0 THEN 555
550 GOTO 570
555 IF H<1 THEN 7050
560 GO TO 755
565 IF ABS(H) +K =0 THEN 7000
570 IF L=1 THEN 580
575 GOTO 600
580 IF K=2 THEN 590
585 GO TO 755
590 IF H=-4 THEN 7050
595 GO TO 755
600 IF L=2 THEN 610
605 GOTO 670
610 IF K=0 THEN 620
615 GOTO 630
620 IF H=-5 THEN 7050
625 GO TO 755
630 IF K=2 THEN 640
635 GOTO 650
640 IF H=4 THEN 7050
645 GO TO 755
650 IF K=3 THEN 660
655 GO TO 755
660 IF H=-3 THEN 7050
665 GO TO 755
670 IF L=4 THEN 680
675 GOTO 705
680 IF K>0 THEN 690
685 GO TO 755
690 IF H<-2 THEN 7050
695 IF H>3 THEN 7050
700 GO TO 755
705 IF L=5 THEN 715
710 GO TO 755
715 IF K>0 THEN 730
720 IF H=-2 THEN 7050
725 GO TO 755
730 IF H>2 THEN 7050
735 IF H<-3 THEN 7050
740 IF H<-1 THEN 750
745 GO TO 755
750 IF H+K =0 THEN 7050
755 LET E = 2
760 LET N = ABS(H)+K
765 IF N-E >0 THEN 700
770 IF N-E<0 THEN 7050
775 IF N-E =0 THEN 7000
780 LET E = E+2
785 GO TO 765

```

Figure A-18. BSMON - BASE CENTERED MONOCLINIC.

```

TRCLN      10:32  CEIR  08/16/67
1000 REM SAVED BY J.R.CULLIPHER ON 6/30/67, PH. 3-5944, Y-12
1010 PRINT"          TRICLINIC"
1020 PRINT
1030 PRINT" VALUES NOT NEEDED ARE: 10-4, 22-2, 21-3, 10-3, 22-1"
1040 PRINT"21-2, 206, 22-0, 211, 23-3, 212, 025, 23-1, 213, 026"
1050 PRINT"04-3, 123, 027, 04-2, 2-4-1, 02-3, 04-1, 2-2-1, 11-2"
1060 PRINT"2-21, 12-2, 031, 120, 033"
1070 PRINT
1080 PRINT "      D", " H", "      K", "      L"
1090 FOR L = -5 TO 6
1100 LET K = 0
1110 FOR H = 1 TO 2
1120 GOSUB 2820
1130 NEXT H
1140 NEXT L
1150 LET L = 0
1160 LET K = 0
1170 FOR H = 3 TO 6
1180 GOSUB 2820
1190 NEXT H
1200 FOR L = 1 TO 7
1210 FOR K = 0 TO 2
1220 LET H = 0
1230 GOSUB 2820
1240 NEXT K
1250 NEXT L
1260 FOR L = -4 TO 0
1270 FOR K = 1 TO 2
1280 LET H = 0
1290 GOSUB 2820
1300 NEXT K
1310 NEXT L
1320 FOR L = -6 TO 4
1330 LET K = 1
1340 LET H = 1
1350 GOSUB 2820
1360 NEXT L
1370 FOR L = -3 TO 5
1380 LET K = -1
1390 LET H = 1
1400 GOSUB 2820
1410 NEXT L
1420 FOR L = -4 TO 2
1430 LET K = 2
1440 LET H = 2
1450 GOSUB 2820
1460 NEXT L
1470 FOR L = -4 TO 0
1480 LET K = 3
1490 LET H = 2
1500 GOSUB 2820
1510 NEXT L
1520 FOR L = -4 TO 3
1530 LET K = 4
1540 LET H = 0
1550 GOSUB 2820
1560 NEXT L
1570 FOR L = -3 TO 2
1580 LET K = -2
1590 LET H = 2
1600 GOSUB 2820
1610 NEXT L
1620 LET L = 3
1630 FOR K = -4 TO -2
1640 LET H = 1
1650 GOSUB 2820
1660 NEXT K
1670 FOR L = -3 TO 2
1680 LET K = 3
1690 LET H = 1
1700 GOSUB 2820
1710 NEXT L
1720 FOR L = 0 TO 4
1730 LET K = 3
1740 LET H = 0
1750 GOSUB 2820
1760 NEXT L
1770 FOR L = -4 TO 4
1780 LET K = 1
1790 LET H = 2
1800 GOSUB 2820
1810 NEXT L
1820 FOR L = -3 TO 2
1830 LET K = -3
1840 LET H = 1
1850 GOSUB 2820
1860 NEXT L
1870 FOR L = -3 TO 4
1880 LET K = 2
1890 LET H = 1
1900 GOSUB 2820
1910 NEXT L
1920 FOR L = -2 TO 1
1930 LET K = -4
1940 LET H = 2
1950 GOSUB 2820
1960 NEXT L
1970 LET H = -4
1980 LET K = 2
1990 LET L = -4
2000 GOSUB 2820
2010 LET L = -2
2020 LET K = 1
2030 LET H = 1
2040 GOSUB 2820
2050 LET K = 5
2060 LET H = 0
2070 GOSUB 2820
2080 LET K = 4
2090 LET H = -2
2100 GOSUB 2820
2110 LET K = 3
2120 LET H = -4
2130 GOSUB 2820
2140 LET L = -1
2150 LET K = 1
2160 LET H = 3
2170 GOSUB 2820
2180 LET K = -1
2190 LET H = 3
2200 GOSUB 2820
2210 LET K = -5
2220 LET H = 1
2230 GOSUB 2820
2240 LET L = 0
2250 LET K = 1
2260 LET H = -4
2270 GOSUB 2820
2280 LET H = -1
2290 GOSUB 2820
2300 LET K = 2
2310 LET H = -2
2320 GOSUB 2820
2330 LET H = -1
2340 GOSUB 2820
2350 LET H = 4
2360 GOSUB 2820
2370 LET K = 3
2380 LET H = -4
2390 GOSUB 2820
2400 LET K = 4
2410 LET H = 2
2420 GOSUB 2820
2430 LET K = 5
2440 LET H = -2
2450 GOSUB 2820
2460 LET K = 6
2470 LET H = 0
2480 GOSUB 2820
2490 LET K = -5
2500 LET H = 1
2510 GOSUB 2820
2520 LET L = 1
2530 LET K = 3
2540 LET H = -1
2550 GOSUB 2820
2560 LET L = 2
2570 LET K = 0
2580 LET H = -2
2590 GOSUB 2820
2600 LET H = 4
2610 GOSUB 2820
2620 LET K = 2
2630 LET H = -4
2640 GOSUB 2820
2650 LET K = 3
2660 LET H = -2
2670 GOSUB 2820
2680 LET L = 4
2690 LET K = 0
2700 LET H = -4
2710 GOSUB 2820
2720 LET K = 1
2730 LET H = -2
2740 GOSUB 2820
2750 PRINT
2760 PRINT
2770 PRINT
2780 PRINT"THE LATTICE PARAMETERS ARE:  A="A, "B="B, "C="C
2790 PRINT"          ALPHA="A7, "BETA="B7, "GAMMA="C7
2800 PRINT
2810 STOP
2820 LET W = A8*(H+2)+B8*(K+2)+C8*(L+2)
2830 LET V8 = 2*D8*H*K + (2*E8*K*L) + 2*F8*H*L
2840 LET U = W+V8
2850 LET D = SQR((V+2)/U)
2860 PRINT D, H,K,L
2870 RETURN
2880 FOR L = 0 TO 0
2890 FOR K = 0 TO 0
2900 FOR H = 0 TO 0

```

Figure A-19. TRCLN - TRICLINIC.

.INTPA 13:43 CEIR 08/17/67			
<u>FACE CENTERED ORTHORHOMBIC</u>			
<u>D</u>	<u>H</u>	<u>K</u>	<u>L</u>
2.595	2	0	0
1.2975	4	0	0
2.753	0	2	0
1.88833	2	2	0
1.17368	4	2	0
1.3765	0	4	0
1.21602	2	4	0
3.20989	1	1	1
1.59302	3	1	1
1.00603	5	1	1
1.66449	1	3	1
1.23284	3	3	1
1.06076	1	5	1
3.046	0	0	2
1.97534	2	0	2
1.19371	4	0	2
2.04242	0	2	2
1.60494	2	2	2
1.09519	4	2	2
1.25437	0	4	2
1.12935	2	4	2
1.78852	1	1	3
1.28077	3	1	3
1.31704	1	3	3
1.06996	3	3	3
1.523	0	0	4
1.31349	2	0	4
1.33266	0	2	4
1.18548	2	2	4
1.02121	0	4	4
1.15955	1	1	5
1.01533	0	0	6
THE LATTICE PARAMETERS ARE: A= 5.19 B= 5.506 C= 6.092			
ALPHA= 90 BETA= 90 GAMMA= 90			
TIME: 17 SECS.			

Figure B-2. LISTING FOR THALLIUM FLUORIDE.

Another discrepancy is that the computer listing of some diffraction reflections do not appear on the ASTM card. All of these except one have the value of d less than 1.16 Å and is, therefore, not on the ASTM card. The one that is above 1.16 Å is the (313) plane. The (400) plane has a value of 1.29750 Å and the (313) has a value of 1.28077 Å. Since a small camera was used, the two lines were very likely merged into a single diffraction line.

The amount of computing time (17 seconds) required for the computer to calculate all of the values is presented at the bottom of the list.