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CRYSTALLOGRAPHIC D-SPACE COMPUTER PROGRAM

by

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CRYSTALLOGRAPHIC D-SPACE COMPUTER PROGRAM

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ABSTRACT

D-Space is a computer program which generates indices $(hk\ell)$, tests for space-group extinctions, and calculates " d ," $1/d^2$, $\sin \theta$, $\sin^2 \theta$, $\sin \theta/\lambda$, $\sin^2 \theta/\lambda^2$, θ , and 2θ for any crystal system and space group, requiring only the unit cell constants as data input. Optional calculations are (1) the single-crystal angle settings, ϕ and χ , and (2) various Lorentz and Lorentz-polarization corrections

INTRODUCTION

A need for a general, crystallographic computer program for calculating interplanar spacings and several basic trigonometric functions essential in diffraction studies exists. Such a program should be very useful for both powder and single-crystal studies involving neutron and/or X-ray diffraction. Because this program started as a joint effort between individuals at Argonne National Laboratory and The University of Texas, it has currently been used on the CDC-1604 and IBM-704 computers. It has been made available to the computer committee of the American Crystallographic Association for listing.

DISCUSSION

The program, which has been written in Fortran, requires only the unit cell constants as input data, with some choice of output with regard to extinctions and various functions.

Indices are incremented in the order of h , then k , then ℓ . The extinction tests are applied, $\sin \theta$ is computed and tested that its value be < 1 , and the output data are calculated and printed before returning to the main program for the next set of indices. Extinctions are ordered in the format found in Buerger.⁽¹⁾

After the positive indices have been generated, negative indices are formed. For the triclinic case, all sign permutations are performed; for

the monoclinic case, only h and $\bar{h}$ are computed. Redundant indices in the cubic, hexagonal, and tetragonal cases can be omitted.

Interplanar spacings and related quantities are computed by means of the general quadratic equation

$$Q = 1/d^2 = (ha^*)^2 + (kb^*)^2 + (lc^*)^2 + 2(klb^*c^*\cos \alpha^* + hla^*c^*\cos \beta^* + hka^*b^*\cos \gamma^*)$$

The reciprocal lattice parameters are computed in the usual way:

$$a^* = (bc \sin \alpha)/V \quad ; \quad b^* = (ac \sin \beta)/V \quad ; \quad c^* = (ab \sin \gamma)/V$$

$$V = abc(1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)^{1/2}$$

$$\cos \alpha^* = (\cos \beta \cos \gamma - \cos \alpha)/(\sin \beta \sin \gamma)$$

$$\cos \beta^* = (\cos \gamma \cos \alpha - \cos \beta)/(\sin \alpha \sin \gamma)$$

$$\cos \gamma^* = (\cos \alpha \cos \beta - \cos \gamma)/(\sin \alpha \sin \beta)$$

The single-crystal angle settings ϕ and χ have the usual meaning as previously described⁽²⁾ and calculated.⁽³⁾ The angle ϕ (ϕ) can be computed for the following 6 different orientations of the crystal:

$$\phi_{c-a} = \tan^{-1} \frac{[V(ck - bl \cos \alpha)]}{bc[bch \sin^2 \alpha + ack(\cos \alpha \cos \beta - \cos \gamma) + abl(\cos \alpha \cos \gamma - \cos \beta)]}$$

$$\phi_{c-b} = \tan^{-1} \frac{[V(ch - al \cos \beta)]}{ac[bch(\cos \alpha \cos \beta - \cos \gamma) + ack \sin^2 \beta + abl(\cos \beta \cos \gamma - \cos \alpha)]}$$

$$\phi_{b-c} = \tan^{-1} \frac{[V(bh - ak \cos \gamma)]}{ab[bch(\cos \alpha \cos \gamma - \cos \beta) + ack(\cos \beta \cos \gamma - \cos \alpha) + abl \sin^2 \gamma]}$$

$$\phi_{b-a} = \tan^{-1} \frac{[V(bl - ck \cos \alpha)]}{bc[bch \sin^2 \alpha + ack(\cos \alpha \cos \beta - \cos \gamma) + abl(\cos \alpha \cos \gamma - \cos \beta)]}$$

$$\phi_{a-b} = \tan^{-1} \frac{[V(al - ch \cos \beta)]}{ca[bch(\cos \alpha \cos \beta - \cos \gamma) + ack \sin^2 \beta + abl(\cos \beta \cos \gamma - \cos \alpha)]}$$

$$\phi_{a-c} = \tan^{-1} \frac{[V(ak - bh \cos \gamma)]}{ba[bch(\cos \alpha \cos \gamma - \cos \beta) + ack(\cos \beta \cos \gamma - \cos \alpha) + abl \sin^2 \gamma]}$$

where the subscripts a , b , and c indicate the relative orientation of the crystal. The first subscript letter indicates the axis of the crystal along

the ϕ axis, and the second subscript letter indicates the reciprocal axis of the crystal in the plane of the χ circle.

The ϕ_{b-a} calculation above would indicate, for example, that the "b" axis was along the ϕ axis, the usual goniometer axis, and that the a^* axis is in the plane of the χ circle, which, with the proper 2θ setting, would be correct for the $h00$ reflections.

Chi can be computed for 3 axial rotations in which the subscript a, b, or c describes the crystal axis - the unique axis - along the ϕ axis of the instrument:

$$\chi_a = \sin^{-1} [(h/a) d_{hkl}]$$

$$\chi_b = \sin^{-1} [(k/b) d_{hkl}]$$

$$\chi_c = \sin^{-1} [(\ell/c) d_{hkl}] \quad .$$

In all of the above it is assumed that $\phi = \chi = 0$ for calculation purposes; however, constant corrections can be added algebraically to phi and chi so that the calculated values correspond to actual goniostat settings.

The following Lorentz or Lorentz-polarization corrections can be computed:

- A. Lorentz correction, crystal face, symmetrical reflection:

$$L = 1/\sin 2\theta$$

- B. Lorentz correction, Debye-Scherrer lines on cylindrical film:

$$L = \frac{1}{2} \sin^2 \theta \cos \theta$$

- C. Lorentz-polarization correction, Debye-Scherrer lines on cylindrical film:

$$L.P. = (1 + \cos^2 2\theta) / \sin^2 \theta \cos \theta$$

- D. Lorentz-polarization correction, equi-inclination Weissenberg photographs:

$$L.P. = \frac{(1 + \cos^2 2\theta)}{\sin 2\theta} \frac{\sin \theta}{(\cos^2 \mu - \cos^2 \theta)^{1/2}}$$

Because $\sin \theta$ and $\sin 2\theta$ are computed and stored in the main program, the L. P. correction is calculated by means of the expression

$$\text{L.P.} = \frac{(2 - \sin^2 2\theta)}{\sin 2\theta} \frac{\sin \theta}{(\cos^2 \mu + \sin^2 \theta - 1)^{1/2}},$$

where:

$$\cos^2 \mu = [1.0 - (n\lambda/2T)]$$

and

T = identity period .

RUNNING TIME

The running time usually varies from 1 to 5 min, depending upon the space group, options chosen, and computer used. The largest problem encountered to date involved over 7000 reflections with phi and chi calculations, and required 40 min on the IBM-704.

FORTRAN NOTATION

<u>Function</u>	<u>Fortran Symbol</u>	<u>Function</u>	<u>Fortran Symbol</u>
$\cos \alpha$	CWA	c^*	CS
$\sin \alpha$	SWA	V (volume)	V
$\cos \beta$	CWB	$Q = 1/d^2$	SUM
$\sin \beta$	SWB	$\sin^2 \theta / \lambda^2$	SQTL S
$\cos \gamma$	CWC	$\sin \theta / \lambda$	SINTL
$\sin \gamma$	SWC	"d"	D
$\cos \alpha^*$	COSAS	θ	THETA
$\cos \beta^*$	COSBS	2θ	TWOTH
$\cos \gamma^*$	COSCS	$\sin 2\theta$	SN2TH
a^*	AS	$\sin \theta$	SINTH
b^*	BS		

All trigonometric functions are calculated by library subroutines.

INPUT CARDS

Card	Columns	Variable	Code Name	Description
1	1 to 72	-	-	Hollerith title card; If program is run under format control, observe limitation for column 1.
2	1 to 10	α	WAD	Lattice constant, decimal point in col. 5
	11 to 20	β	WBD	Lattice constant, decimal point in col. 15
	21 to 30	γ	WCD	Lattice constant, decimal point in col. 25
	31 to 40	a	A	Lattice constant, decimal point in col. 35
	41 to 50	b	B	Lattice constant, decimal point in col. 45
	51 to 60	c	C	Lattice constant, decimal point in col. 55
	61 to 70	λ	XL	Wavelength of radiation, in Å; decimal point in col. 64.

Note: All angles should be expressed as degrees and decimal fractions of degrees.

Card

3	Column 1	LA(HKL)
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$h + k + \ell = 2n$, condition for non-extinction
	4	$h + k = 2n$
	5	$h + \ell = 2n$
	6	$k + \ell = 2n$
	7	$h + k = 2n$, $h + \ell = 2n$, and $k + \ell = 2n$
	8	$-h + k + \ell = 3n$
	9	$h + k + \ell = 3n$
	Column 2	LB(OKL)
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$k = 2n$

	4	$\ell = 2n$
	5	$k + \ell = 2n$
	6	$k + \ell = 4n$
Column 3	LC(HOL)	
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$h = 2n$
	4	$\ell = 2n$
	5	$h + \ell = 2n$
	6	$h + \ell = 4n$
Column 4	LD(HKO)	
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$h = 2n$
	4	$k = 2n$
	5	$h + k = 2n$
	6	$h + k = 4n$
Column 5	LE(HHL)	
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$\ell = 2n$
	4	$h = 2n$
	5	$h + \ell = 2n$
	6	$2h + \ell = 4n$
Column 6	LF(HOO)	
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$h = 2n$
	4	$h = 4n$

Column 7	LG(OKO)	
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$k = 2n$
	4	$k = 4n$
Column 8	LH(OOL)	
	1	omit this and all succeeding tests
	2	omit this test, go to next test
	3	$\ell = 2n$
	4	$\ell = 3n$
	5	$\ell = 4n$
	6	$\ell = 6n$
Column 9	LI(HHO)	
	1	omit this test
	2	$h = 2n$
Column 10	NP(PHI)	
	0	omit this calculation
	1	calculate ϕ_{c-a}
	2	calculate ϕ_{c-b}
	3	calculate ϕ_{b-c}
	4	calculate ϕ_{b-a}
	5	calculate ϕ_{a-b}
	6	calculate ϕ_{a-c}
Column 11	NC(CHI)	
	0	omit this calculation
	1	calculate χ_c
	2	calculate χ_b
	3	calculate χ_a

Column 12 LP(COR)

- 0 omit L or LP calculations
- 1 L for crystal face, symmetrical reflection
- 2 L for Debye-Scherrer Lines on cylindrical film
- 3 LP for Debye-Scherrer lines on cylindrical film
- 4 LP, equi-inclination, a-axis rotation
- 5 LP, equi-inclination, b-axis rotation
- 6 LP, equi-inclination, c-axis rotation

Column 13 NCT

- 0 all values of h , k , and ℓ are computed, with specified extinctions
- 1 criteria $h \geq k \geq \ell$ must be satisfied.
(Cubic case: $h \geq 0, k \geq 0, \ell \geq 0$)
- 2 criteria $h \geq k$ must be satisfied. (Tetragonal or hexagonal case: $h \geq k, h \geq 0, k \geq 0$)

Columns 14-20: Should be punched 0 or 1 for sign permutation control.

Column 14

- 0 omit this sign permutation and proceed to next possibility
- 1 calculate $\bar{h}k\ell$

Column 15

- 0 omit
- 1 calculate $h\bar{k}\ell$

Column 16

- 0 omit
- 1 calculate $\bar{h}\bar{k}\ell$

Column 17

0	omit
1	calculate $hk\bar{\ell}$

Column 18

0	omit
1	calculate $\bar{h}k\bar{\ell}$

Column 19

0	omit
1	calculate $h\bar{k}\bar{\ell}$

Column 20

0	omit
1	calculate $\bar{\bar{h}}\bar{\bar{k}}\bar{\bar{\ell}}$

Columns 21-30: (ADJP) correction to ϕ to be added algebraically to calculated values. Decimal point in col. 25

Columns 31-40: (ADJC) correction to χ to be added algebraically to calculated values. Decimal point in col. 35

Note: In card 3, columns 1-9 must have punches (not 0) in them, otherwise a "computational error" at relative address xxxxxx will occur. If column 10 is zero, column 11 must also be zero.

In card 3, columns 14-20 are used to control the sign permutation of $hk\ell$. If columns 14-20 are punched zero only the $hk\ell$ case is computed. For example, the following may apply: Monoclinic and hexagonal systems; 14-20, 1000000, orthorhombic, tetragonal and cubic systems and hexagonal powder patterns; 14-20, 0000000.

CARD DECK ARRANGEMENT

IBM-704

D-Space binary program deck

Card 1. (Title card)

Card 2. (Cell constants card)

Card 3. (Options card)

Blank card

Blank card

Note 1: When using with the CDC-1604, the deck arrangement may vary according to the compiler system in operation for each computer. The output mode may have to be changed to meet the demands of the individual system, e.g., the WRITE TAPE statement may have to be changed to PRINT.

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

1209/MET 135

704 PROGRAM

GENERAL OPERATING INSTRUCTIONS

Programmer

Date

USED

NOT USED

Meyer and Janousek6/21/61DRUM: ☐☒UP SWITCH: ☒☐

READER: 72 x 72 board

PUNCH: Not used

PRINTER: Not used

SENSE SWITCH SETTINGS: All up

TAPES:

Input: None

Scratch: None

Output - Printed #2

- Punched

To Be Saved

None

Rewound by Program Prior to Calculation None After None

Manual EOF Needed

TIME BEFORE OUTPUT:

a few seconds

NORMAL RUNNING TIME: Approx. 30 sec. to 5 min. depending on

RUN NO LONGER THAN: 45 mins.

sign permutations and
extinction choices.

RUNNING PROCEDURE: (Indicate both regular and restart)

1. READY tape #2.
2. SET underflow switch on.
3. READY binary program deck followed by data cards in reader.
4. CLEAR and LOAD CARDS.
5. HPR 77777₈ in S.R. - problem completed.
6. Write EOF on tape #2, remove, and print off-line.

STOPS (OCTAL): HPR 77777 - End of problem.

HPR 777 - Illegal negative values for NP and/or LP. Press
START to read next case.

HPR 77 - Illegal negative values for NP, LP, and/or NC.

Press START to continue without calculating ϕ , χ , or LP.

AMD-5 (12-61)

FORTRAN Error Stops

TEST PROBLEM - ALPHA URANIUM

The test problem selected for this program (MET-135) was that of alpha uranium, which is orthorhombic Space group No. 63, Cmc₂m, which has the following conditions for the reflections:

$$\begin{array}{ll}
 hk\ell: h + k = 2n & h00: (h = 2n) \\
 0k\ell: (k = 2n) & 0k0: (k = 2n) \\
 h0\ell: \ell = 2n \quad ; \quad (h = 2n) & 00\ell: (\ell = 2n) \\
 hk0: (h + k = 2n)
 \end{array}$$

The lattice constants are indicated in Fig. 1, which is the data sheet used for punching the necessary 3 cards. It can be noted from this sheet that the calculation is for $\text{CuK}\alpha$ radiation and that the $hk\ell$ output has been limited based upon the above reflection conditions. In this test case, one of the options is also being used, namely, the calculation of ϕ and χ based on the b axis of the crystal unique - b axis along the ϕ axis - and the a^* axis of the crystal is in the plane of the χ circle.

The output from an IBM-704 run is shown in Fig. 2. The title and input information, under identifying symbols, are printed on the first few lines, thereby affording a convenient check on input data. The next 2 lines list the unit cell volume, cosines of the reciprocal lattice angles, and the reciprocal lattice parameters. The last portion is a columnar arrangement of the output data in which the following abbreviations are used for column headings:

D	d spacing
1/DSQ	$1/d^2$
SINTH	$\sin\theta$
SINTHS	$\sin^2\theta$
SINTL	$\sin\theta/\lambda$
SQTL	$\sin^2\theta/\lambda^2$
THETA	θ
2THETA	2θ
PHI	ϕ
CHI	χ
LP	Lorentz-polarization correction

FIGURE 2. MET-135 704 OUTPUT SHEET - ALPHA URANIUM
TEST PROGRAM

1209/MET135 ALPHA URANIUM B AXIS UNIQUE 5/3/62											
ALPHA			BETA			GAMMA			A		
90.00000			90.00000			90.00000			2.85390		
									5.86910		
									4.95540		
									1.541780		
HKL	OKL	HOL	HKO	HHL	HGO	CKO	COL	HMO	PHI	CHI	COR
4	3	4	5	1	3	3	3	1	4	2	0

SOURCE DECK LISTING

```

C      1209/MET135   D SPACE
      DIMENSION FS(3),INDX(7)                                4
      COMMON SINTH,XL,LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,         6
      1NC,V,A,B,C,BCMA,CAMB,ABMC,CWA,CWB,CWC,SWA,SWB,SWC,LP,NCT,ALPHAP, 8
      2ND,MPP,MPC,ADJP,ADJC
      10 FORMAT(6F10.5,F10.6)                                10
      101 FORMAT( 93H0  H   K   L   D           1/DSQ      SINTH      SINTHS  12
      1   SINTL      SQTLS      THETA      2THETA      )      14
      107 FORMAT(94H           V           COSA*           COSB*           COSG*  16
      X           A*           R*           C*)           18
      108 FORMAT (F16.5,6F13.6///)                          20
      109 FORMAT(106H      ALPHA      BETA      GAMMA      A      B      22
      X   C   LAMBDA      )      24
      110 FORMAT (6F10.5, F10.6 ///)                          26
      111 FORMAT(109H0  H   K   L   D           1/DSQ      SINTH      SINTHS  28
      1   SINTL      SQTLS      THETA      2THETA      PHI      CHI      )  30
      123 FORMAT(22H01209/MET135   D SPACE)                  32
      710 FORMAT(112H  HKL OKL HOL HKO HHL HOO OKO OOL HHO PHI CHI COR NCT -36
      1KL H-L --L HK- -K- H-- ---          ADJPHI      ADJCHI      )      38
      781 FORMAT(100H0  H   K   L   D           1/DSQ      SINTH      SINTHS  40
      1   SINTL      SQTLS      THETA      2THETA      L-LP      )      42
      1231 FORMAT (72H                                     44
      1                                     )      46
      1998 FORMAT(20(3X,1I1),6X,F10.5,5X,F10.5 ///)         48
      1999 FORMAT (20I1,2F10.5)                              50
      1233 READ 1231                                         52
      WRITE OUTPUT TAPE 2,123
      777 READ 10, WAD, WBD,WCD,A,B,C,XL                      56
      WRITE OUTPUT TAPE 2,1231
      IF (A) 778,18,778                                     60
      778 READ 1999, LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,NC,LP,NCT,(INDX(NA),NA= 62
      11,7),ADJP,ADJC
      WRITE OUTPUT TAPE 2,109
      WRITE OUTPUT TAPE 2,110,WAD,WBD,WCD,A,B,C,XL          66
      WRITE OUTPUT TAPE 2,710
      WRITE OUTPUT TAPE 2,1998,LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,NC,LP,NCT, 70
      1(INDX(NA),NA=1,7),ADJP,ADJC                          71
      WA = WAD/57.2957895                                     72
      WB = WBD/57.2957895                                     74
      WC = WCD/57.2957895                                     76
      CWA = COSF(WA)                                          COSA
      CWB = COSF(WB)                                          COSB
      CWC = COSF(WC)                                          COSB
      SWA = SINF(WA)                                          SINA
      SWB = SINF(WB)                                          SINB
      SWC = SINF(WC)                                          SINB
      BCMA=CWB*CWC-CWA                                         90
      CAMB=CWC*CWA-CWB                                         92
      ABMC=CWA*CWB-CWC                                         94
      COSAS=BCMA/(SWB*SWC)                                     96
      COSBS=CAMB/(SWC*SWA)                                     98
      COSCS=ABMC/(SWA*SWB)                                    100
      NA=0                                                     109
      V = A*B*C*SQRTF(1.0+2.0*CWA*CWB*CWC-CWA*CWA-CWB*CWB-CWC*CWC)  VOLUM

```

AS = B*C*SWA/V	A*
BS = A*C*SWB/V	B*
CS = A*B*SWC/V	C*
WRITE OUTPUT TAPE 2,107	
WRITE OUTPUT TAPE 2,108,V,COSAS,COSBS,COSCS,AS,BS,CS	
761 IF(NP) 82,762,779	114
762 IF(LP) 82,765,782	116
779 WRITE OUTPUT TAPE 2,111	
780 GO TO 783	120
765 WRITE OUTPUT TAPE 2,101	
766 GO TO 783	124
782 WRITE OUTPUT TAPE 2,781	
783 FS (1) = 1.	128
FS (2) = 1.	130
FS (3) = 1.	132
21 FH=1.0	134
FK=0.0	136
FL=0.0	138
3 CALL HKL (FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)	140
IF (SINTH - 1.0) 2,4,4	142
2 FH = FH+ 1.0	144
GO TO 3	146
4 FK = FK + 1.0	148
CALL HKL (FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)	150
IF (SINTH - 1.0) 5,6,6	152
5 FH = 0.0	154
GO TO 3	156
6 FH = 0.0	158
CALL HKL (FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)	160
IF (SINTH - 1.0) 2,8,8	162
8 FH = 0.0	164
FK = 0.0	166
FL = FL + 1.0	168
CALL HKL (FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)	170
IF (SINTH - 1.0) 2,9,9	172
9 FH = FH + 1.0	174
CALL HKL(FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)	176
IF (SINTH - 1.0) 2,20,20	178
20 FH = 0.0	180
FK = FK + 1.0	182
CALL HKL(FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)	184
IF (SINTH - 1.0) 2,16,16	186
16 NA=NA+1	188
GO TO (31,32,33,34,35,36,37,15),NA	
31 IF(INDX(1)) 12,16,12	
12 FS(1)=-1.0	
FS(2)=1.0	
FS(3)=1.0	
GO TO 21	
32 IF(INDX(2)) 13,16,13	
13 FS(1)=1.0	
FS(2)=-1.0	
FS(3)=1.0	
GO TO 21	

33 IF(INDX(3)) 14,16,14

14 FS(1)=-1.0

FS(2)=-1.0

FS(3)=1.0

GO TO 21

34 IF(INDX(4)) 17,16,17

17 FS(1)=1.0

FS(2)=1.0

FS(3)=-1.0

GO TO 21

35 IF(INDX(5)) 19,16,19

19 FS(1)=-1.0

FS(2)=1.0

FS(3)=-1.0

GO TO 21

36 IF(INDX(6)) 22,16,22

22 FS(1)=1.0

FS(2)=-1.0

FS(3)=-1.0

GO TO 21

37 IF (INDX(7)) 23,16,23

23 FS(1)=-1.0

FS(2)=-1.0

FS(3)=-1.0

GO TO 21

82 PAUSE 777

15 GO TO 1233

18 STOP 77777

END (0,1,0,0,1)

218

220

222

```

C      1209/MET135      SUBROUTINE HKL
      SUBROUTINE HKL (FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,FS)
      DIMENSION FS(3)
      COMMON SINTH,XL,LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,
      INC,V,A,B,C,BCMA,CAMB,ABMC,CWA,CWB,CWC,SWA,SWB,SWC,LP,NCT,ALPHAP,
      2ND,MPP,MPC,ADJP,ADJC
1711  FORMAT(3I4,8F10.5)
711   FORMAT(3I4,9F10.5)
11    FORMAT (3I4, 10F10.5 )
      FHS = FS(1)*FH
      FKS = FS(2)*FK
      FLS = FS(3)*FL
      SUM = (FHS*AS)**2 + (FKS*BS)**2 + (FLS*CS)**2 + 2.0*(FKS*FLS*BS*CS*
      1COSAS +FHS*FLS*CS*AS*COSBS + FHS*FKS*AS*BS*COSCS)
      SQTLS = SUM/4.0
      SINTL = SQRTF(SQTLS)
      SINTH = SINTL*XL
      CHI = -0.0

C      IF (SINTH - 1.0) 49,50,50
49     SINTHS=SINTH**2
      IF (NCT-1) 2000,600,610
600    IF(FH-FK)50,605,605
605    IF(FK-FL)50,2000,2000
610    IF(FH-FK)50,2000,2000
2000   GO TO (33,2003,1001,1055,1056,1057,1004,1002,1003),LA
1001   A7 = ABSF(FHS + FKS + FLS)
      IF (A7) 121,2003,121
121    IF (A7-2.0)50,2003,123
123    A7 = A7-2.0
      GO TO 121
1055   FE=ABSF(FHS+FKS)
751    IF (FE) 752,2003,752
752    IF (FE-2.0)50,2003,753
753    FE=FE-2.0

C      GO TO 752
1056   FI=ABSF(FHS+FLS)
761    IF (FI) 762,2003,762
762    IF (FI-2.0)50,2003,763
763    FI=FI-2.0
      GO TO 762
1057   FO=ABSF(FKS+FLS)
771    IF (FO) 772,2003,772
772    IF (FO-2.0)50,2003,773
773    FO=FO-2.0
      GO TO 772
1004   DA=ABSF(FHS+FKS)
      IF (DA) 141,145,141
141    IF (DA-2.0)50,145,142
142    DA=DA-2.0
      GO TO 141
145    E=ABSF(FHS+FLS)
140    IF (E) 146,2003,146

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146 IF (E-2.0)50,2003,147	330
147 E=E-2.0	332
GO TO 146	334
1002 B7 = ABSF(-FHS+FKS+FLS)	K+L-H=3N
IF (B7) 143,2003,143	338
143 IF (B7) 50,2003,144	340
144 B7 = B7-3.0	342
GO TO 143	344
1003 C7 = ABSF(FHS+FKS+FLS)	H+K+L=3N
IF (C7)131,2003,131	348
131 IF (C7-3.0)50,2003,132	350
132 C7 = C7-3.0	362
GO TO 131	354
2003 IF(FH) 2005,2004,2005	356
2004 GO TO(33,2005,1009,1010,1011,1012),L8	358
1009 P=FK	K=2N
IF (P) 161,2005,161	362
161 IF (P-2.0)50,2005,162	364
162 P=P-2.0	366
GO TO 161	368
1010 QA = FL	L=2N
IF (QA) 163,2005,163	372
163 IF (QA-2.0) 50,2005,164	374
164 QA=QA-2.0	376
GO TO 163	378
1011 R=ABSF(FKS+FLS)	K+L=2N
IF (R) 165, 2005, 165	382
165 IF(R-2.0)50,2005,166	384
166 R=R-2.0	386
GO TO 165	388
1012 S=ABSF(FKS+FLS)	K+L=4N
IF (S) 167,2005,167	392
167 IF(S-4.0)50,2005,168	394
168 S=S-4.0	396
GO TO 167	398
2005 IF(FK) 2007,2006,2007	400
2006 GO TO (33,2007,1027,1026,1024,1025),LC	402
1027 AC=FH	H=2N
IF (AC) 187,2007,187	406
187 IF(AC-2.0)50,2007,188	408
188 AC=AC-2.0	410
GO TO 187	412
1026 AB=FL	L=2N
IF (AB) 185,2007,185	416
185 IF(AB-2.0)50,2007,186	418
186 AB=AB-2.0	420
GO TO 185	422
1024 Z=ABSF(FHS+FLS)	H+L=2N
IF (Z) 181,2007,181	426
181 IF(Z-2.0)50,2007,182	428
182 Z=Z-2.0	430
GO TO 181	432
1025 AA=ABSF(FHS+FLS)	H+L=4N
IF (AA) 183,2007,183	436

183 IF(AA-4.0)50,2007,184	438
184 AA=AA-4.0	440
GO TO 183	442
2007 IF (FL) 2001,2008,2001	444
2008 GO TO (33,2001,1030,1031,1032,1033),LD	446
1030 AF=FH	H=2N
IF (AF) 195,2001,195	450
195 IF (AF-2.0)50,2001,196	452
196 AF=AF-2.0	454
GO TO 195	456
1031 AG=FK	K=2N
IF (AG) 197,2001,197	460
197 IF (AG-2.0)50,2001,198	462
198 AG=AG-2.0	464
GO TO 197	466
1032 AH=ABSF(FHS+FKS)	H+K=2N
IF (AH) 199,2001,199	470
199 IF (AH-2.0)50,2001,200	472
200 AH=AH-2.0	474
GO TO 199	476
1033 AI=ABSF(FHS+FKS)	H+K=4N
IF (AI) 201,2001,201	480
201 IF (AI-4.0) 50,2001,202	482
202 AI=AI-4.0	484
GO TO 201	486
2001 IF (FHS-FKS)1028,2002,1028	488
2002 GO TO (33,1028,1005,1006,1007,1008),LE	490
1005 F = FL	L=4N
IF (F) 151,1028,151	494
151 IF (F-2.0) 50,1028,152	496
152 F = F - 2.0	498
GO TO 151	500
1006 G=FH	H=2N
IF (G) 153,1028,153	504
153 IF (G-2.0) 50,1028,154	506
154 G=G-2.0	508
GO TO 153	510
1007 H=ABSF(FHS+FLS)	H+L=2N
IF (H) 155,1028,155	514
155 IF (H-2.0) 50,1028,156	516
156 H=H-2.0	518
GO TO 155	520
1008 O=ABSF(FHS+FHS+FLS)	2H+L=4N
IF (O) 157,1028,157	524
157 IF (O-4.0) 50,1028,158	526
158 O = O-4.0	528
GO TO 157	530
1028 IF (FL) 1013,1029,1013	532
1029 IF (FK) 1013,2009,1013	534
2009 GO TO (33,1013,189,192),LF	536
189 AD = FH	H=2N
IF (AD) 190,1013,190	540
190 IF (AD-2.0)50,1013,191	542
191 AD=AD-2.0	544

GO TO 190	546
192 AE=EH	548
193 IF (AE-4.0)50,1013,194	H=4N
194 AE=AE-4.0	552
GO TO 193	554
1013 IF (FL) 1017,2050,1017	556
2050 IF (FH) 1017,2051,1017	558
2051 GO TO (33,1017,1015,1016), LG	560
1015 T=FK	K=2N
IF (T) 169,1017,169	564
C	566
169 IF (T-2.0)50,1017,170	568
170 T=T-2.0	570
GO TO 169	572
1016 U=FK	K=4N
IF (U) 171,1017,171	576
171 IF (U-4.0)50,1017,172	578
172 U=U-4.0	580
GO TO 171	582
1017 IF (FK) 1034,2055,1034	00L
2055 IF (FH) 1034,1018,1034	586
1018 GO TO (33,1034,1019,1020,1021,1022),LH	588
1019 V=FL	L=2N
IF (V) 173,1034,173	592
173 IF (V-2.0) 50,1034,174	594
174 V=V-2.0	596
GO TO 173	598
1020 W = FL	L=3N
IF (W) 175,1034,175	602
175 IF (W-3.0) 50,1034,176	604
176 W=W-3.0	606
GO TO 175	608
1021 X=FL	L=4N
IF (X) 177,1034,177	612
177 IF (X-4.0) 50,1034,178	614
178 X=X-4.0	616
GO TO 177	618
1022 Y=FL	L=6N
IF (Y) 179,1034,179	622
179 IF (Y-6.0) 50,1034,180	624
180 Y=Y-6.0	626
GO TO 179	628
1034 IF (FH-FK)33,2060,33	HHO
2060 IF (FL) 33,2061,33	H=2N
2061 GO TO (33,1035), LI	634
1035 AJ=EH	636
IF (AJ) 203,33,203	638
203 IF(AJ-2.0)50,33,204	640
204 AJ=AJ-2.0	642
GO TO 203	644
33 D = 1.0/SCRTF(SUM)	646
750 THETA=ASINF(SINTH)	648
TWOTH=THETA*2.0	650
SN2TH = SINF(TWOTH)	652

1965 IF(LP)998,890,1966	654
1966 GO TO (1967,1969,1972,1974,1977,1980), LP	656
1967 SLP = 1.0 / SN2TH	658
1968 GO TO 45	660
1969 SLP=1.0/(SINTHS*2.0*COSF(THETA))	662
1970 GO TO 45	664
1972 SLP=(1.0+COSF(TWOTH)**2)/(SINTHS*COSF(THETA))	666
1973 GO TO 45	668
1974 COSQMU = 1.0 - ((FH*XL)/(2.0*A))**2	670
GO TO 1975	672
1977 COSQMU = 1.0 - ((FK*XL)/(2.0*B))**2	674
GO TO 1975	676
1980 COSQMU = 1.0 - ((FL*XL)/(2.0*C))**2	678
C EQUI INCLINATION LP CORRECTION	680
1975 SLP = (2.0-SN2TH*SN2TH)*SINTH/(SN2TH*SQRTF(COSQMU+SINTHS-1.0))	682
GO TO 45	684
890 IF(NP)998, 45,900	686
900 GO TO (905,910,915,920,925,930),NP	PHI
905 TNPCA=(V*(C*FKS-B*FLS*CWA))/(B*C*(	690
1B*C*FHS*SWA**2+A*C*FKS*ABMC+A*B*FLS*CAMB))	692
PHI=ATANF(TNPCA)*57.2957895	694
909 GO TO 940	696
910 TNPBC=(V*(C*FHS-A*FLS*CWb))/(A*C*(B*C*	698
1FHS*ABMC+A*C*FKS*SWB**2+A*B	700
2*FLS*BCMA))	702
PHI=ATANF(TNPBC)*57.2957895	704
914 GO TO 940	706
915 TNPBC=(V*(B*FHS-A*FKS*CWc))/(A*B*(B*	708
1C*FHS*CAMB+A*C*FKS*BCMA+A*B*FLS*SWC**2))	710
PHI=ATANF(TNPBC)*57.2957895	712
919 GO TO 940	714
920 TNPBA=(V*(B*FLS-C*FKS*CWA))/(B*C*(B*	716
1C*FHS*SWA**2+A*C*FKS*ABMC+A*B*FLS*CAMB))	718
PHI=ATANF(TNPBA)*57.2957895	720
924 GO TO 940	722
925 TNPAB=(V*(A*FLS-C*FHS*CWb))/(A*C*(B	724
1C*FHS*ABMC+A*C*FKS*SWB**2+A*B*FLS*BCMA))	726
PHI=ATANF(TNPAB)*57.2957895	728
929 GO TO 940	730
930 TNPAC=(V*(A*FKS-B*FHS*CWc))/(B*A*(B*C	732
1*FHS*CAMB+A*C*FKS*BCMA+A*B*FLS*SWC**2))	734
PHI=ATANF(TNPAC)*57.2957895	736
940 PHI = PHI + ADJP	738
949 IF(NC)998,45, 950	CHI
950 GO TO (955,960,965),NC	742
955 SNCC=FLS*D/C	744
IF (ABSF(SNCC)-1.) 22222,22221,22221	746
22222 CHI=ASINF(SNCC)*57.2957895	748
959 GO TO 35	750
960 SNCB=FKS*D/B	752
IF (ABSF(SNCB)-1.) 22223,22221,22221	754
22223 CHI=ASINF(SNCB)*57.2957895	756
964 GO TO 35	758
965 SNCA=FHS*D/A	760

IF (ABSF(SNCA)-1.) 22224,22221,22221	762
22224 CHI=ASINF(SNCA)*57.2957895	764
GO TO 35	766
C	768
22221 CHI = 90.	770
35 CHI = CHI + ADJC	772
45 ISA = FHS	774
KSA = FKS	776
LSA = FLS	778
THETA=THETA*57.2957895	780
TWOTH = THETA*2.0	782
970 IF(NP)996,975,996	784
975 IF(LP)977,980,977	786
980 WRITE OUTPUT TAPE 2,1711,ISA,KSA,LSA,D,SUM,SINTH,SINTHS,SINTL, ISQTLS,THETA,TWOTH	
985 GO TO 50	790
977 WRITE OUTPUT TAPE 2, 711,ISA,KSA,LSA,D,SUM,SINTH,SINTHS,SINTL, ISQTLS,THETA,TWOTH,SLP	
GO TO 50	796
996 WRITE OUTPUT TAPE 2, 11,ISA,KSA,LSA,D,SUM,SINTH,SINTHS,SINTL, ISQTLS,THETA,TWOTH,PHI,CHI	
997 GO TO 50	802
998 PAUSE 77	804
GO TO 45	806
50 RETURN	808
END (0,1,0,0,1)	

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REFERENCES

1. M. J. Buerger, X-ray Crystallography, John Wiley and Sons, Inc., New York (1942), p. 83.
2. T. C. Furnas and D. Harker, Rev. Sci. Instr. 26, 449 (1955).
3. B. T. M. Willis, Use of a Two-circle Device to Obtain Three-dimensional Neutron Diffraction Data, AERE-R-3308 (March 1960).