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CRYSTALLOGRAPHIC D-SPACE COMPUTER PROGRAM

by

M. H. Mueller, E. F. H. Meyer,
and S. H. Simonsen

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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, phi and chi, 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

$$Q = 1/d^2 = (ha^*)^2 + (kb^*)^2 + (\ell c^*)^2$$
$$+ 2(k\ell b^*c^*\cos\alpha^* + h\ell a^*c^*\cos\beta^* + hka^*b^*\cos\gamma^*) \quad .$$

The reciprocal lattice parameters are computed in the usual way:

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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:

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

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 θ and sin 2θ 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

$$T = \text{identity period} .$$

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

Function	Fortran Symbol	Function	Fortran Symbol
$\cos \alpha$	CWA	c^*	CS
$\sin \alpha$	SWA	V (volume)	V
$\cos \beta$	CWB	$Q = 1/d^2$	SUM
$\sin \beta$	SWB	$\sin^2 \theta/\lambda^2$	SQTLS
$\cos \gamma$	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 $h \geqq k \geqq \ell$ must be satisfied. (Cubic case: $h \geqq 0$, $k \geqq 0$, $\ell \geqq 0$)
2	criteria $h \geqq k$ must be satisfied. (Tetragonal or hexagonal case: $h \geqq k$, $h \geqq 0$, $k \geqq 0$)

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 $\bar{h}\bar{k}\bar{\ell}$

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 xxxxx 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
Meyer and Janousek	6/21/61

	USED	NOT USED
DRUM:		X
UF SWITCH:	X	

READER: 72 × 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 sign permutations and extinction choices.

RUN NO LONGER THAN: 45 mins.

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 77777_8 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.

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, Cmcm, which has the following conditions for the reflections:

$hk\ell$: $h + k = 2n$	$h00$: $(h = 2n)$
$0k\ell$: $(k = 2n)$	$0k0$: $(k = 2n)$
$h0\ell$: $\ell = 2n$; $(h = 2n)$	00ℓ: $(\ell = 2n)$
$hk0$: $(h + k = 2n)$	

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 CuK_α 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	$\sin\theta/\lambda$
SQTLS	$\sin^2\theta/\lambda^2$
THETA	θ
2THETA	2θ
PHI	ϕ
CHI	χ
LP	Lorentz-polarization correction

704 INPUT DATA

FORM II

COST CODE 1209

FIGURE 1. MET-135 704 DATA SHEET - ALPHA URANIUM TEST PROBLEM

PROGRAM MET 135 PROBLEM Alpha Uranium ORIGINATOR Mueller DATE 2/28/62 PAGE 1 OF 1

1	2	3	4	5	6	7	8
1209/	MET 135 ALPHA URANIUM BAXIS UNIQUE	2/28/61					
90.00	90.00	90.00	2.8539	5.8691	4.9554	1.54178	
4345133314200							

AMD-9 (9-60)

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	B	C	LAMBDA
90.00000	90.00000	90.00000	2.85390	5.86910	4.95540	1.541780

HKL	OKL	HOL	HKO	HHL	HOO	OKO	OOL	HHO	PHI	CHI	COR	NCT	-KL	H-L	--L	HK-	-K-	H--	---	ADJPHI	ADJCHI
4	3	4	5	1	3	3	3	1	4	2	0	0	0	0	0	0	0	0	0	-0.	-0.

V	COSA*	COSB*	COSG*	A*	B*	C*
83.00208	-0.000000	-0.000000	-0.000000	0.350398	0.170384	0.201800

H	K	L	D	1/DSQ	SINTH	SINTHS	SINTL	SQTLS	THETA	2THETA	PHI	CHI
2	0	0	1.42695	0.49111	0.54024	0.29186	0.35040	0.12278	32.69972	65.39944	0.	0.
1	1	0	2.56656	0.15181	0.30036	0.09022	0.19481	0.03795	17.47920	34.95840	-0.00001	25.93174
3	1	0	0.93904	1.13404	0.82093	0.67393	0.53246	0.28351	55.17801	110.35601	-0.00000	9.20679
0	2	0	2.93455	0.11612	0.26269	0.06901	0.17038	0.02903	15.23000	30.46001	45.00001	90.00000
2	2	0	1.28328	0.60724	0.60072	0.36086	0.38963	0.15181	36.92142	73.84284	-0.00001	25.93174
1	3	0	1.61363	0.38405	0.47774	0.22823	0.30986	0.09601	28.53771	57.07541	-0.00002	55.56913
3	3	0	0.85552	1.36628	0.90108	0.81194	0.58444	0.34157	64.30022	128.60044	-0.00001	25.93174
0	4	0	1.46728	0.46449	0.52539	0.27603	0.34077	0.11612	31.69443	63.38886	45.00001	90.00000
2	4	0	1.02297	0.95560	0.75358	0.56789	0.48878	0.23890	48.90178	97.80356	-0.00001	44.20177
1	5	0	1.08558	0.84854	0.71012	0.50427	0.46058	0.21214	45.24443	90.48887	-0.00003	67.64247
0	6	0	0.97818	1.04510	0.78808	0.62108	0.51115	0.26128	52.00676	104.01352	45.00001	90.00000
2	6	0	0.80681	1.53622	0.95547	0.91293	0.61972	0.38405	72.83792	145.67585	-0.00002	55.56913
1	7	0	0.80444	1.54528	0.95829	0.91832	0.62155	0.38632	73.39311	146.78622	-0.00005	73.62785
1	1	1	2.27902	0.19253	0.33826	0.11442	0.21939	0.04813	19.77060	39.54120	29.93839	22.84928
3	1	1	0.92263	1.17476	0.83554	0.69813	0.54193	0.29369	56.67209	113.34418	10.86700	9.04444
0	2	1	2.52501	0.15685	0.30530	0.09321	0.19802	0.03921	17.77631	35.55261	-89.99998	59.36633
2	2	1	1.24230	0.64796	0.62054	0.38506	0.40248	0.16199	38.35524	76.71048	16.06421	25.04534
1	3	1	1.53433	0.42478	0.50243	0.25243	0.32587	0.10619	30.16072	60.32145	29.93838	51.65378
3	3	1	0.84305	1.40701	0.91441	0.83614	0.59309	0.35175	66.12190	132.24380	10.86700	25.52629
0	4	1	1.40690	0.50521	0.54794	0.30023	0.35539	0.12630	33.22555	66.45110	-89.99996	73.50620
2	4	1	1.00184	0.99633	0.76947	0.59209	0.49908	0.24908	50.30662	100.61323	16.06420	43.06208
1	5	1	1.06043	0.88927	0.72696	0.52847	0.47151	0.22232	46.63191	93.26381	29.93838	64.60922
0	6	1	0.95967	1.08583	0.80329	0.64528	0.52102	0.27146	53.44551	106.89102	-89.99993	78.83355
2	6	1	0.79633	1.57694	0.96806	0.93713	0.62788	0.39424	75.47886	150.95773	16.06420	54.49742
1	7	1	0.79405	1.58600	0.97083	0.94252	0.62968	0.39650	76.12784	152.25567	29.93837	71.27197
0	0	2	2.47770	0.16289	0.31113	0.09680	0.20180	0.04072	18.12742	36.25484	-90.00000	0.
2	0	2	1.23654	0.65401	0.62342	0.38866	0.40435	0.16350	38.56663	77.13325	29.93839	0.
1	1	2	1.78258	0.31470	0.43246	0.18702	0.28049	0.07868	25.62355	51.24710	49.03614	17.68140
3	1	2	0.87810	1.29693	0.87791	0.77073	0.56941	0.32423	61.39145	122.78291	21.00404	8.60452
0	2	2	1.89315	0.27902	0.40720	0.16581	0.26411	0.06975	24.02900	48.05801	-89.99999	40.17509
2	2	2	1.13951	0.77013	0.67651	0.45767	0.43879	0.19253	42.57154	85.14307	29.93839	22.84928
1	3	2	1.35216	0.54695	0.57012	0.32504	0.36978	0.13674	34.75850	69.51699	49.03614	43.72181
3	3	2	0.80867	1.52918	0.95328	0.90875	0.61830	0.38229	72.41718	144.83437	21.00403	24.41564
0	4	2	1.26251	0.62738	0.61060	0.37284	0.39604	0.15685	37.63313	75.26625	-89.99998	59.36633
2	4	2	0.94555	1.11850	0.81529	0.66469	0.52880	0.27962	54.61564	109.23129	29.93838	40.12243
1	5	2	0.99433	1.01144	0.77529	0.60107	0.50285	0.25286	50.83099	101.66197	49.03614	57.89643
0	6	2	0.90984	1.20800	0.84728	0.71788	0.54954	0.30200	57.91671	115.83342	-89.99997	68.45617
1	1	3	1.38900	0.51832	0.55500	0.30802	0.35997	0.12958	33.71052	67.42104	59.93832	13.68967
3	1	3	0.81635	1.50055	0.94432	0.89173	0.61248	0.37514	70.78941	141.57883	29.93839	7.99534
0	2	3	1.43943	0.48263	0.53555	0.28681	0.34736	0.12066	32.38126	64.76252	-89.99999	29.37431
2	2	3	1.01339	0.97375	0.76070	0.57867	0.49339	0.24344	49.52623	99.05246	40.82295	20.20201
1	3	3	1.15427	0.75056	0.66786	0.44604	0.43318	0.18764	41.90220	83.80440	59.93833	36.15740
0	4	3	1.09698	0.83100	0.70274	0.49384	0.45580	0.20775	44.64702	89.29404	-89.99998	48.38570
2	4	3	0.86969	1.32211	0.88639	0.78569	0.57492	0.33053	62.42356	124.84713	40.82295	36.35071
1	5	3	0.90720	1.21505	0.84975	0.72207	0.55115	0.30376	58.18429	116.36858	59.93833	50.61140
0	6	3	0.84167	1.41161	0.91590	0.83888	0.59406	0.35290	66.33453	132.66905	-89.99998	59.36633
0	0	4	1.23885	0.65157	0.62226	0.38721	0.40360	0.16289	38.48155	76.96311	-90.00000	0.
2	0	4	0.93548	1.14269	0.82405	0.67907	0.53448	0.28567	55.49275	110.98550	49.03614	0.
1	1	4	1.11568	0.80338	0.69096	0.47743	0.44816	0.20085	43.70620	87.41239	66.53483	10.95825
0	2	4	1.14132	0.76769	0.67544	0.45622	0.43809	0.19192	42.48832	84.97665	-90.00000	22.88754
2	2	4	0.89129	1.25881	0.86491	0.74807	0.56098	0.31470	59.87274	119.74548	49.03614	17.68140
1	3	4	0.98265	1.03563	0.78450	0.61544	0.50883	0.25891	51.67463	103.34927	66.53483	30.15114
0	4	4	0.94658	1.11606	0.81440	0.66324	0.52822	0.27902	54.52789	109.05577	-89.99999	40.17509
2	4	4	0.78880	1.60718	0.97729	0.95510	0.63387	0.40179	77.76635	155.53271	49.03614	32.52020
1	5	4	0.81646	1.50012	0.94418	0.89148	0.61240	0.37503	70.76588	141.53176	66.53484	44.07204
1	1	5	0.92454	1.16989	0.83381	0.69523	0.54081	0.29247	56.49172	112.98345	70.84933	9.06340
0	2	5	0.93898	1.13420	0.82099	0.67402	0.53250	0.28355	55.18405	110.36811	-90.00000	18.66127
2	2	5	0.78439	1.62532	0.98279	0.96588	0.63744	0.40633	79.35541	158.71082	55.21833	15.50331
1	3	5	0.84451	1.40214	0.91282	0.83325	0.59206	0.35053	65.89869	131.79737	70.84934	25.57378
0	4	5	0.82128	1.48257	0.93864	0.88105	0.60880	0.37064	69.82485	139.64970	-89.99999	34.03731
0	0	6	0.82590	1.46604	0.93339	0.87122	0.60540	0.36651	68.97020	137.94040	-90.00000	0.
1	1	6	0.78620	1.61785	0.98053	0.96144	0.63597	0.40446	78.67538	157.35076	73.85993	7.69822
0	2	6	0.79501	1.58216	0.96966	0.94023	0.62892	0.39554	75.64924	151.69849	-90.00000	15.71873

1209/MET135 D SPACE

SOURCE DECK LISTING

```
C     1209/MET135   D SPACE
      DIMENSION FS(3),INDX(7)
      COMMON SINTH,XL,LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,
     1NC,V,A,B,C,BCMA,CAMB,ABMC,CWA,CWB,CWC,SWA,SWB,SWC,LP,NCT,ALPHAP,
     2ND,MPP,MPC,ADJP,ADJC
   10 FORMAT(6F10.5,F10.6)
  101 FORMAT( 93H0  H   K   L    D          1/DSQ     SINTH    SINTHS
     1  SINTL     SQTLS    THETA     2THETA   )
  107 FORMAT(94H                V        COSA*        COSB*        COSG*
     X          A*            B*          C*)
  108 FORMAT (F16.5,6F13.6///)
  109 FORMAT(106H     ALPHA      BETA     GAMMA          A          B
     X    C    LAMBDA                                    )
  110 FORMAT (6F10.5, F10.6 //)
  111 FORMAT(109H0  H   K   L    D          1/DSQ     SINTH    SINTHS
     1  SINTL    SQTLS     THETA     2THETA    PHI       CHI    )
  123 FORMAT(22H01209/MET135   D SPACE)
  710 FORMAT(112H  HKL OKL HOL HKO HHL HOO OKO OOL HHO PHI CHI COR NCT -
     1KL H-L --L HK- -K- H-- ---          ADJPHI          ADJCHI      )
  781 FORMAT(100H0  H   K   L    D          1/DSQ     SINTH    SINTHS
     1  SINTL     SQTLS    THETA     2THETA    L-LP    )
 1231 FORMAT (72H
     1                        )
 1998 FORMAT(20(3X,1I1),6X,F10.5,5X,F10.5 ///)
 1999 FORMAT (20I1,2F10.5)
 1233 READ 1231
      WRITE OUTPUT TAPE 2,123
  777 READ 10, WAD, WBD,WCD,A,B,C,XL
      WRITE OUTPUT TAPE 2,1231
      IF (A) 778,18,778
  778 READ 1999, LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,NC,LP,NCT,(INDX(NA),NA=
     11,7),ADJP,ADJC
      WRITE OUTPUT TAPE 2,109
      WRITE OUTPUT TAPE 2,110,WAD,WBD,WCD,A,B,C,XL
      WRITE OUTPUT TAPE 2,710
      WRITE OUTPUT TAPE 2,1998,LA,LB,LC,LD,LE,LF,LG,LH,LI,NP,NC,LP,NCT,
     1(INDX(NA),NA=1,7),ADJP,ADJC
      WA = WAD/57.2957895
      WB = WBD/57.2957895
      WC = WCD/57.2957895
      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
      CAMB=CWC*CWA-CWB
      ABMC=CWA*CWB-CWC
      COSAS=BCMA/(SWB*SWC)
      COSBS=CAMB/(SWC*SWA)
      COSCS=ABMC/(SWA*SWB)
      NA=0
      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                                                    218
15 GO TO 1233                                                   220
18 STOP 77777                                                   222
   END (0,1,0,0,1)
```

```
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,
     1NC,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
```

```
 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),LB                          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
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                                                                      438
  183 IF(AA-4.0)50,2007,184                                           440
  184 AA=AA-4.0                                                       442
      GO TO 183                                                       444
 2007 IF (FL)     2001,2008,2001                                      446
 2008 GO TO (33,2001,1030,1031,1032,1033),LD                          H=2N
 1030 AF=FH                                                           450
      IF (AF)     195,2001,195                                        452
  195 IF (AF-2.0)50,2001,196                                          454
  196 AF=AF-2.0                                                       456
      GO TO 195                                                       K=2N
 1031 AG=FK                                                           460
      IF (AG)     197,2001,197                                        462
  197 IF (AG-2.0)50,2001,198                                          464
  198 AG=AG-2.0                                                       466
      GO TO 197                                                       H+K=2N
 1032 AH=ABSF(FHS+FKS)                                                470
      IF (AH)     199,2001,199                                        472
  199 IF (AH-2.0)50,2001,200                                          474
  200 AH=AH-2.0                                                       476
      GO TO 199                                                       H+K=4N
 1033 AI=ABSF(FHS+FKS)                                                480
      IF (AI)     201,2001,201                                        482
  201 IF (AI-4.0) 50,2001,202                                         484
  202 AI=AI-4.0                                                       486
      GO TO 201                                                       488
 2001 IF (FHS-FKS)1028,2002,1028                                      490
 2002 GO TO (33,1028,1005,1006,1007,1008),LE                          L=4N
 1005 F = FL                                                          494
      IF (F)     151,1028,151                                        496
  151 IF (F-2.0) 50,1028,152                                          498
  152 F = F - 2.0                                                     500
      GO TO 151                                                       H=2N
 1006 G=FH                                                            504
      IF (G)     153,1028,153                                        506
  153 IF (G-2.0) 50,1028,154                                          508
  154 G=G-2.0                                                         510
      GO TO 153                                                       H+L=2N
 1007 H=ABSF(FHS+FLS)                                                 514
      IF (H)     155,1028,155                                        516
  155 IF (H-2.0) 50,1028,156                                          518
  156 H=H-2.0                                                         520
      GO TO 155                                                       2H+L=4N
 1008 O=ABSF(FHS+FHS+FLS)                                             524
      IF (O)     157,1028,157                                        526
  157 IF (O-4.0) 50,1028,158                                          528
  158 O = O-4.0                                                       530
      GO TO 157                                                       532
 1028 IF (FL)     1013,1029,1013                                      534
 1029 IF (FK)     1013,2009,1013                                      536
 2009 GO TO (33,1013,189,192),LF                                      H=2N
  189 AD = FH                                                         540
      IF (AD)     190,1013,190                                        542
  190 IF (AD-2.0)50,1013,191                                          544
  191 AD=AD-2.0
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      GO TO 190                                                         546
  192 AE=FH                                                             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                                        OOL
 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                                              HH0
 2060 IF (FL)     33,2061,33                                            H=2N
 2061 GO TO (33,1035), LI                                               634
 1035 AJ=FH                                                             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/SQRTF(SUM)                                                646
  750 THETA=ASINF(SINTH)                                                648
      TWOTH=THETA*2.0                                                   650
      SN2TH = SINF(TWOTH)                                               652
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 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 TNPCB=(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(TNPCB)*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
     1*C*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
22224 CHI=ASINF(SNCA)*57.2957895
      GO TO 35
C
22221 CHI = 90.
   35 CHI = CHI + ADJC
   45 ISA = FHS
      KSA = FKS
      LSA = FLS
      THETA=THETA*57.2957895
      TWOTH = THETA*2.0
  970 IF(NP)996,975,996
  975 IF(LP)977,980,977
  980 WRITE OUTPUT TAPE 2,1711,ISA,KSA,LSA,D,SUM,SINTH,SINTHS,SINTL,
     1SQTLS,THETA,TWOTH
  985 GO TO 50
  977 WRITE OUTPUT TAPE 2, 711,ISA,KSA,LSA,D,SUM,SINTH,SINTHS,SINTL,
     1SQTLS,THETA,TWOTH,SLP
      GO TO 50
  996 WRITE OUTPUT TAPE 2,  11,ISA,KSA,LSA,D,SUM,SINTH,SINTHS,SINTL,
     1SQTLS,THETA,TWOTH,PHI,CHI
  997 GO TO 50
  998 PAUSE 77
      GO TO 45
   50 RETURN
      END (0,1,0,0,1)
```

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