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and Space Administration

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PROGRAMS FOR CALCULATING CELL PARAMETERS
IN ELECTRON AND X-RAY DIFFRACTION

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SUMMARY

Ten programs for calculating cell parameters from single-crystal electron diffraction patterns are presented. Most of the programs, written for use with a programmable desk calculator, are also applicable to x-ray diffraction work. The programs can be used to calculate d-spacings from electron diffraction plate measurements, and to determine cell data (including interplanar angles and zone angles) for all crystal systems. A program for rhombohedral-hexagonal conversions and one for matching crystal data from standards with apparent crystal parameters found in diffraction patterns are included. Because they allow rapid determination of data not present in x-ray listings or elsewhere in the literature, the programs facilitate identification of unknowns. Full understanding of the programs requires some knowledge of crystal structure and familiarity with programming the HP-97 calculator. The programs are easy and inexpensive to use compared to the time required on large computers. Furthermore, data appear immediately so that results are available continuously while working on a problem.

INTRODUCTION

For more than a year we have been using the selected-area, single-crystal electron diffraction method to identify stratospheric aerosols and associated particulate matter. Initially we made use of poorly oriented crystals that gave rise to only a few disorganized, apparently unrelated reflections. The amount of information obtained by examining a grain in only one orientation is limited, especially if the orientation is an irrational one. But by combining d-spacing data from a number of differently oriented particles of, presumably, the same substance, we have had some success in identification, using as comparative data the well-known Joint Committee on Powder Diffraction Standards (JCPDS) file of compounds. Our possibilities for unknowns are limited to a relatively few sulfate compounds, and this restriction helps in identification, although admittedly some unsuspected phases might go unrecognized. This initial approach can be compared with the use of powder x-ray patterns in conjunction with the JCPDS standard file, except that with electron diffraction, extra reflections may appear to confuse the comparison with x-ray data, and

intensities of electron reflections are not generally comparable to x-ray intensities.

ORIENTED PATTERNS

Even though we have not had access to a tilt stage for our RCA EMU 4 instrument, with the consequence that orientation of a single crystal cannot be adjusted at will, many of our patterns are oriented so that a well-populated lattice layer is in the plane of the grid-supported film used as the collection surface, giving rise to symmetrically disposed reflection patterns having an apparent symmetry center on the plate. In the course of evaluation of these oriented patterns, we made use of the traditional formulas for determination of interplanar spacings (appendix). We also found that, in interpreting the patterns, calculation of cell parameters for the various crystal systems is important. But as work progressed, and we began to employ interplanar angles and axial ratios as well as d spacings as identification criteria, the formulas became difficult to solve manually. Accordingly, a series of short programs, designed for use with an HP-97 calculator, was devised. The HP-97 is a small programmable desk calculator having a maximum of 224 programming steps and 26 storage registers. This capacity is limited relative even to modest commercial units, such as the CDC 7600 or IBM 360 computers, but the capability is perfectly adequate for the purpose, and expenses are of course much lower than with larger units. Cost of the HP-97 is \$750.00 at time of writing; there is also a nominal expense for printout paper and magnetic input cards. The small calculator allows one to have results at hand immediately while working on a problem, and avoids the turnaround time for a large computer.

DESCRIPTION OF PROGRAMS

The programs listed here range from simple (Program 1: calculation of camera constant and d spacings in electron diffraction patterns) to complex (Program 9: determination of triclinic crystal-system parameters). For full understanding of the programs, some familiarity with crystal structure and electron or x-ray diffraction is required. Although the programs were designed for use with an HP-97 calculator, workers with some knowledge of the style of programming used can perhaps adapt the program steps to other units.

It is assumed in using most of the programs that one is dealing with electron diffraction of an oriented crystal; that is, that a principal plane of symmetry of the crystal is perpendicular to the electron beam. Lacking a tilt stage, one must trust to luck to obtain such an orientation; but minerals often lie on cleavages that are parallel to simple rational indices and, as noted above, we have found that many of the crystals we encounter in aerosols have grown or been deposited so that they are lying on a major crystal plane.

Program 10 involves calculation of apparent crystallographic parameters, such as may be observed in diffraction patterns of nonorthogonal crystals, from the known parameters of standard compounds. This is a reverse procedure

to that of the other programs and requires some explanation. In oriented or unoriented diffraction patterns of orthogonal (cubic, tetragonal, and orthorhombic) crystals, the d-spacing value of a plane that intersects only one axis always reflects the value of the cell edge corresponding to that axis. For example, if a diffraction spot is known to correspond to (001) in an unoriented pattern of an orthorhombic crystal, the value of d obtained by measurement approximates the cell edge of the compound; and, if the pattern is oriented, then another cell edge should be obtainable. But even in oriented patterns of nonorthogonal crystals, some or all of the d spacings known to represent planes (100), (010), or (001) may be less than the actual values of the lengths of the axes that they intersect. For instance, in a monoclinic crystal having its a and b crystallographic axes in a plane perpendicular to the electron beam, (100) reflections may be observed, but the a axis cannot be estimated directly from the value of $d_{(100)}$, and will be larger than $d_{(100)}$, owing to the geometry introduced by the β crystallographic angle. Similar cases can be cited for the other nonorthogonal systems (i.e., hexagonal, rhombohedral, and triclinic). In addition, it can be shown that in the rhombohedral and triclinic systems, all crystallographic axial angles measured from the disposition of electron diffraction spots in an oriented pattern are the apparent, and not the true, axial angles. This is the case even if the orientation is a simple one, but the situation is not easily visualized and must be demonstrated by use of the formulas (appendix). The only instances where it is possible to measure an axial angle in the spot pattern of a nonorthogonal crystal are the (010) orientation of a monoclinic crystal, which yields the β axial angle — and of course the (001) orientation of a hexagonal crystal, which gives the 120° interaxial angle. We would also point out that while an axial angle of 90° , as measured on an electron diffraction plate, suggests the simple orientation of a compound belonging to an orthogonal crystal system, the pattern may in fact be referable to any nonorthogonal system except the rhombohedral, the exception being due to the fact that no orientation of any rhombohedral lattice can give rise to even apparent angles of 90° .

Given these complications, program 10 is presented in order to facilitate comparison of experimental diffraction data with standard (e.g., JCPDS) data, thus allowing changes to known standard values of cell edges and axial angles to synthesize observed (100), (010), and (001) d spacings of diffraction patterns and their apparent interplanar angles. Thus a whole set of possible mineral compounds can be gone through and data generated for comparison with the unknown. We have found this convenient in instances in which there is some knowledge of what the unknown might be. Program 10 is also useful in verifying solutions arrived at by other means and, in addition, allows one to infer various kinds of cells and thus examine the data that would be produced by them in an experimental electron diffraction pattern.

The 10 programs, in approximate order of increasing complexity, are described below. Formulas used in the calculations and input and output values are included. Because it is a general case of the other systems, the triclinic program (program 9) could be used for most of the more symmetrical classes, treating these as special examples of the triclinic. Our experience has shown, however, that it is more convenient to reserve programs for each

crystal system. It should be noted that most of the programs can be used for x-ray diffraction data.

Program 1: Electron Diffraction Experimental d Calculation

Program use- This program is used to calculate camera constant of plates, and d spacings of electron diffraction spots. It is assumed the sample has a thin layer of gold evaporated on it for calibration purposes. The plate is centered on a reader which has a centimeter measurement scale, and the scale reading is noted at points opposed to each other on the innermost gold ring (2.355 Å). The program calculates the camera constant (k) and location of the center of the diffraction pattern (stored in Register 3). Scale readings of diffraction spots can then be used to calculate d (for single spots) or d_{ave} (for a pair of corresponding spots). The applicable formulas are:

$$k = (d_{gold})(\text{diameter}_{gold \text{ ring}})$$

$$d_{(unknown)} = (k/2)(\text{reading at diffraction spot} \\ - \text{reading at center diffraction pattern})$$

$$d_{ave(unknown)} = k/(\text{reading at diffraction spot 1} \\ - \text{reading at diffraction spot 2})$$

The input and output parameters:

	Input parameters	Output parameters
Label A Calculate k	Reading at one side of gold ring ENTER Reading at other side of gold ring	k
Label B Calculate d	Reading at diffraction spot	d Distance of spot from center
Label C Calculate d_{ave}	Reading at diffraction spot 1 of pair ENTER Reading at diffraction spot 2 of pair	d_{ave} Average distance of diffraction spots from center

Program 1 can be executed as many times as desired by entering the indicated input parameters as listed, and then pushing the appropriate label button (e.g., push A for label A). Subprogram A must be run before subprograms B and C can be executed, but it need be run only once before a series of subprograms B and C is executed; if the camera constant changes, subprogram A must be run once before any series of subprograms B or C. The actual program follows.

Camera Constant and d-spacing Calculation

ØØ1	*LBLA	21 11	Ø26	STOØ	35 ØØ	Ø51	STOB	35 12
ØØ2	STO4	35 Ø4	Ø27	RCL3	36 Ø3	Ø52	-	-45
ØØ3	X≐Y	-41	Ø28	-	-45	Ø53	RCL1	36 Ø1
ØØ4	STO5	35 Ø5	Ø29	2	Ø2	Ø54	X≐Y	-41
ØØ5	+	-55	Ø3Ø	x	-35	Ø55	÷	-24
ØØ6	2	Ø2	Ø31	RCL1	36 Ø1	Ø56	ABS	16 31
ØØ7	÷	-24	Ø32	X≐Y	-41	Ø57	DSP4	-63 Ø4
ØØ8	STO3	35 Ø3	Ø33	÷	-24	Ø58	1	Ø1
ØØ9	RCL4	36 Ø4	Ø34	ABS	16 31	Ø59	X>Y?	16-34
Ø1Ø	RCL5	36 Ø5	Ø35	DSP4	-63 Ø4	Ø6Ø	DSP5	-63 Ø5
Ø11	-	-45	Ø36	1	Ø1	Ø61	X≐Y	-41
Ø12	2	Ø2	Ø37	X>Y?	16-34	Ø62	PRTX	-14
Ø13	.	-62	Ø38	DSP5	-63 Ø5	Ø63	RCLA	36 11
Ø14	3	Ø3	Ø39	X≐Y	-41	Ø64	RCLB	36 12
Ø15	5	Ø5	Ø4Ø	PRTX	-14	Ø65	+	-55
Ø16	5	Ø5	Ø41	RCLØ	36 ØØ	Ø66	2	Ø2
Ø17	x	-35	Ø42	RCL3	36 Ø3	Ø67	÷	-24
Ø18	ABS	16 31	Ø43	-	-45	Ø68	RCLA	36 11
Ø19	STO1	35 Ø1	Ø44	ABS	16 31	Ø69	-	-45
Ø2Ø	SPC	16-11	Ø45	DSP4	-63 Ø4	Ø7Ø	ABS	16 31
Ø21	FIX	-11	Ø46	PRTX	-14	Ø71	DSP4	-63 Ø4
Ø22	DSP6	-63 Ø6	Ø47	RTN	24	Ø72	PRTX	-14
Ø23	PRTX	-14	Ø48	*LBLC	21 13	Ø73	RTN	24
Ø24	RTN	24	Ø49	STOA	35 11	Ø74	R/S	51
Ø25	*LBLB	21 12	Ø5Ø	X≐Y	-41			

Program 2: Cubic System Crystal Parameters

Program use- This program is used to calculate d spacings, angles (ϕ) between planes, angles (ρ) between crystal zones, and cell edge for the cubic crystal system. The applicable formulas are:

$$d^2 = \frac{a^2}{h^2 + k^2 + l^2}$$

$$a = d(h^2 + k^2 + l^2)^{1/2}$$

$$\cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{(h_1^2 + k_1^2 + l_1^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}}$$

$$\cos\rho = \frac{u_1u_2 + v_1v_2 + w_1w_2}{(u_1^2 + v_1^2 + w_1^2)^{1/2}(u_2^2 + v_2^2 + w_2^2)^{1/2}}$$

The Input and output parameters are:

	Input parameters	Output parameters ^a	
Label A	Register 1- a	d	or d
Calculate d	Register 4- h	hkl	h
	Register 5- k		k
	Register 6- l		l
Label B	Register 4- h	a	
Calculate a	Register 5- k		
	Register 6- l		
	Register D- d		
Label C	Register 1- a	d	
Calculate all possible d's within limits	Register 7- largest h to be printed	hkl	
	Register 8- largest k to be printed		
NOTE: $h < k < l$	Register 9- largest l to be printed		
Reg. 7 < 8 < 9	Register E- only d values larger than this printed		
Label D	Register 4- $h_1 (u_1)$	$\phi (\rho)$	$\phi (\rho)$
Calculate angle (ϕ) between crystal planes	Register 5- $k_1 (v_1)$	$h_1 k_1 l_1 (u_1 v_1 w_1)$	$h_1 (u_1)$
or	Register 6- $l_1 (w_1)$	$h_2 k_2 l_2 (u_2 v_2 w_2)$	$k_1 (v_1)$
Calculate angle (ρ) between crystal zones	Register 7- $h_2 (u_2)$		$l_1 (w_1)$
	Register 8- $k_2 (v_2)$		$h_2 (u_2)$
	Register 9- $l_2 (w_2)$		$k_2 (v_2)$
			$l_2 (w_2)$

^aIf h, k, and l (u, v, and w) are zero or positive and less than 10, output is in the form hkl (uvw). If h, k, or l (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h & u \\ k & v \\ l & w \end{matrix}$ (vertical rather than horizontal format).

The programs can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push A for Label A). The actual program follows.

Cubic Calculations

001	*LBLA	21	11	052	RCL6	36	06	103	√X	54
002	GSB1	23	01	053	RCL5	36	05	104	RCLA	36 11
003	÷	-24		054	X=Y?	16-33		105	X⇒Y	-41
004	√X	54		055	GTOc	22	16 13	106	÷	-24
005	DSP4	-63	04	056	RCL8	36	08	107	COS ⁻¹	16 42
006	PRTX	-14		057	X=Y?	16-33		108	DSP2	-63 02
007	GSB2	23	02	058	GTOc	22	16 13	109	PRTX	-14
008	RTN	24		059	X⇒Y	-41		110	GSB2	23 02
009	*LBLB	21	12	060	1	01		111	9	09
010	SPC	16-11		061	+	-55		112	RCL7	36 07
011	RCLD	36	14	062	STO5	35	05	113	X>Y?	16-34
012	GSBa	23	16 11	063	STO6	35	06	114	GTO9	22 09
013	√X	54		064	GTO7	22	07	115	X<0?	16-45
014	x	-35		065	*LBLc	21	16 13	116	GTO9	22 09
015	DSP4	-63	04	066	RCL5	36	05	117	9	09
016	PRTX	-14		067	RCL4	36	04	118	RCL8	36 08
017	RTN	24		068	X=Y?	16-33		119	X>Y?	16-34
018	*LBLC	21	13	069	R/S	51		120	GTO9	22 09
019	RCL9	36	09	070	RCL7	36	07	121	X<0?	16-45
020	RCL8	36	08	071	X=Y?	16-33		122	GTO9	22 09
021	X>Y?	16-34		072	R/S	51		123	9	09
022	R/S	51		073	X⇒Y	-41		124	RCL9	36 09
023	RCL7	36	07	074	1	01		125	X>Y?	16-34
024	X>Y?	16-34		075	+	-55		126	GTO9	22 09
025	R/S	51		076	STO4	35	04	127	X<0?	16-45
026	0	00		077	STO5	35	05	128	GTO9	22 09
027	STO4	35	04	078	STO6	35	06	129	RCL7	36 07
028	STO5	35	05	079	GTO7	22	07	130	1	01
029	STO6	35	06	080	*LBLD	21	14	131	0	00
030	*LBL0	21	00	081	RCL4	36	04	132	0	00
031	RCL9	36	09	082	RCL7	36	07	133	x	-35
032	RCL6	36	06	083	x	-35		134	+	-55
033	X=Y?	16-33		084	RCL5	36	05	135	RCL8	36 08
034	GTOb	22	16 12	085	RCL8	36	08	136	1	01
035	1	01		086	x	-35		137	0	00
036	+	-55		087	+	-55		138	x	-35
037	STO6	35	06	088	RCL6	36	06	139	+	-55
038	*LBL7	21	07	089	RCL9	36	09	140	DSP0	-63 00
039	GSBd	23	16 14	090	x	-35		141	PRTX	-14
040	÷	-24		091	+	-55		142	RTN	24
041	√X	54		092	STOA	35	11	143	*LBL1	21 01
042	RCL5	36	15	093	RCL7	36	07	144	SPC	16-11
043	X>Y?	16-34		094	X ²	53		145	*LBLd	21 16 14
044	GTOb	22	16 12	095	RCL8	36	08	146	RCL1	36 01
045	X⇒Y	-41		096	X ²	53		147	X ²	53
046	SPC	16-11		097	+	-55		148	*LBLa	21 16 11
047	DSP4	-63	04	098	RCL9	36	09	149	RCL4	36 04
048	PRTX	-14		099	X ²	53		150	X ²	53
049	GSB2	23	02	100	+	-55		151	RCL5	36 05
050	GTO0	22	00	101	GSBa	23	16 11	152	X ²	53
051	*LBLb	21	16 12	102	x	-35		153	+	-55

Cubic Calculations (Concluded)

154	RCL6	36 06	173	X>Y?	16-34	192	RCL4	36 04
155	X ²	53	174	GTO8	22 08	193	DSP0	-63 00
156	+	-55	175	X<0?	16-45	194	PRTX	-14
157	RTN	24	176	GTO8	22 08	195	RCL5	36 05
158	*LBL2	21 02	177	RCL4	36 04	196	PRTX	-14
159	9	09	178	1	01	197	RCL6	36 06
160	RCL4	36 04	179	0	00	198	PRTX	-14
161	X>Y?	16-34	180	0	00	199	RTN	24
162	GTO8	22 08	181	x	-35	200	*LBL9	21 09
163	X<0?	16-45	182	+	-55	201	RCL7	36 07
164	GTO8	22 08	183	RCL5	36 05	202	DSP0	-63 00
165	9	09	184	1	01	203	PRTX	-14
166	RCL5	36 05	185	0	00	204	RCL8	36 08
167	X>Y?	16-34	186	x	-35	205	PRTX	-14
168	GTO8	22 08	187	+	-55	206	RCL9	36 09
169	X<0?	16-45	188	DSP0	-63 00	207	PRTX	-14
170	GTO8	22 08	189	PRTX	-14	208	RTN	24
171	9	09	190	RTN	24	209	R/S	51
172	RCL6	36 06	191	*LBL8	21 08			

Program 3: Tetragonal System Crystal Parameters

Program use- This program is used to calculate d spacings of crystal planes, interplanar angles (ϕ), interzonal angles (ρ), and cell edges for the tetragonal crystal system. The applicable formulas are:

$$d = \frac{ac}{[c^2(h^2 + k^2) + a^2l^2]^{1/2}}$$

$$a = d_1 d_2 \left[\frac{1_2^2(h_1^2 + k_1^2) - 1_1^2(h_2^2 + k_2^2)}{d_2^2 l_2^2 - d_1^2 l_1^2} \right]^{1/2}$$

$$c = adl \left[\frac{1}{a^2 - d^2(h^2 + k^2)} \right]^{1/2}$$

$$\cos\phi = \frac{(h_1 h_2 + k_1 k_2)/a^2 + l_1 l_2/c^2}{[(h_1^2 + k_1^2)/a^2 + l_1^2/c^2]^{1/2} [(h_2^2 + k_2^2)/a^2 + l_2^2/c^2]^{1/2}}$$

$$\cos\rho = \frac{a^2(u_1 u_2 + v_1 v_2) + c^2 w_1 w_2}{[a^2(u_1^2 + v_1^2) + c^2 w_1^2]^{1/2} [a^2(u_2^2 + v_2^2) + c^2 w_2^2]^{1/2}}$$

Vertical lines in the formulas imply absolute values.

The input and output parameters are:

	Input parameters	Output parameters ^a	
Label A	Register 1- a	d	or d
Card 1	Register 3- c	hkl	h
Calculate d	Register 4- h		k
	Register 5- k		l
	Register 6- l		
Label B	Register 4- h ₁	a	
Card 3	Register 5- k ₁	c	
Calculate a, c	Register 6- l ₁		
	Register 7- h ₂		
	Register 8- k ₂		
	Register 9- l ₂		
	Register D- d ₁		
	Register E- d ₂		
Label C	Register 1- a	d	
Card 1	Register 3- c	hkl	
Calculate all possible d's within limits	Register 7- largest h to be printed		
	Register 8- largest k to be printed		
NOTE: h < k	Register 9- largest l to be printed		
Reg. 7 < 8	Register E- only d values larger than this printed		
Label D	Register 1- a	φ	or φ
Card 2	Register 3- c	h ₁ k ₁ l ₁	h ₁
Calculate angle (φ) between crystal planes	Register 4- h ₁	h ₂ k ₂ l ₂	k ₁
	Register 5- k ₁		l ₁
	Register 6- l ₁		h ₂
	Register 7- h ₂		k ₂
	Register 8- k ₂		l ₂
	Register 9- l ₂		
Label E	Register 1- a	ρ	or ρ
Card 2	Register 3- c	u ₁ v ₁ w ₁	u ₁
Calculate angle (ρ) between crystal zones	Register 4- u ₁	u ₂ v ₂ w ₂	v ₁
	Register 5- v ₁		w ₁
	Register 6- w ₁		u ₂
	Register 7- u ₂		v ₂
	Register 8- v ₂		w ₂
	Register 9- w ₂		

^aIf h, k, and l (u, v, and w) are zero or positive and less than 10, output is in the form hkl (uvw). If h, k, or l (u, v, w) are negative, or greater than 9, output is in the form $\begin{matrix} h & u \\ k & v \\ l & w \end{matrix}$ (i.e., vertical rather than horizontal format).

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push A for Label A). The actual program follows.

Card 1. Tetragonal

ØØ1	*LBLA	21 11	Ø47	STOA	35 11	Ø93	X=Ø?	16-43
ØØ2	GSB5	23 Ø5	Ø48	STO4	35 Ø4	Ø94	GTO4	22 Ø4
ØØ3	FIX	-11	Ø49	STO5	35 Ø5	Ø95	*LBLc	21 16 13
ØØ4	DSP4	-63 Ø4	Ø5Ø	STO6	35 Ø6	Ø96	RCL5	36 Ø5
ØØ5	SPC	16-11	Ø51	*LBLØ	21 ØØ	Ø97	RCL4	36 Ø4
ØØ6	PRTX	-14	Ø52	RCL9	36 Ø9	Ø98	X=Y?	16-33
ØØ7	*LBL1	21 Ø1	Ø53	RCL6	36 Ø6	Ø99	R/S	51
ØØ8	FIX	-11	Ø54	X=Y?	16-33	1ØØ	RCL7	36 Ø7
ØØ9	DSPØ	-63 ØØ	Ø55	GTOb	22 16 12	1Ø1	X=Y?	16-33
Ø1Ø	9	Ø9	Ø56	1	Ø1	1Ø2	R/S	51
Ø11	RCL4	36 Ø4	Ø57	+	-55	1Ø3	X≠Y	-41
Ø12	X>Y?	16-34	Ø58	STO6	35 Ø6	1Ø4	1	Ø1
Ø13	GTO8	22 Ø8	Ø59	*LBL7	21 Ø7	1Ø5	+	-55
Ø14	X<Ø?	16-45	Ø6Ø	Ø	ØØ	1Ø6	STO4	35 Ø4
Ø15	GTO8	22 Ø8	Ø61	STOA	35 11	1Ø7	STO5	35 Ø5
Ø16	9	Ø9	Ø62	GSB5	23 Ø5	1Ø8	Ø	ØØ
Ø17	RCL5	36 Ø5	Ø63	RCLE	36 15	1Ø9	STO6	35 Ø6
Ø18	X>Y?	16-34	Ø64	X>Y?	16-34	11Ø	GTO7	22 Ø7
Ø19	GTO8	22 Ø8	Ø65	GTOe	22 16 15	111	*LBL2	21 Ø2
Ø2Ø	X<Ø?	16-45	Ø66	X≠Y	-41	112	RCL4	36 Ø4
Ø21	GTO8	22 Ø8	Ø67	SPC	16-11	113	X ²	53
Ø22	9	Ø9	Ø68	FIX	-11	114	RCL5	36 Ø5
Ø23	RCL6	36 Ø6	Ø69	DSP4	-63 Ø4	115	X ²	53
Ø24	X>Y?	16-34	Ø7Ø	PRTX	-14	116	+	-55
Ø25	GTO8	22 Ø8	Ø71	GSB1	23 Ø1	117	RTN	24
Ø26	X<Ø?	16-45	Ø72	GTOØ	22 ØØ	118	*LBL5	21 Ø5
Ø27	GTO8	22 Ø8	Ø73	*LBLe	21 16 15	119	RCL3	36 Ø3
Ø28	RCL4	36 Ø4	Ø74	1	Ø1	12Ø	X ²	53
Ø29	1	Ø1	Ø75	STOA	35 11	121	GSB2	23 Ø2
Ø3Ø	Ø	ØØ	Ø76	*LBLb	21 16 12	122	x	-35
Ø31	Ø	ØØ	Ø77	RCL6	36 Ø6	123	RCL1	36 Ø1
Ø32	x	-35	Ø78	X=Ø?	16-43	124	RCL6	36 Ø6
Ø33	+	-55	Ø79	GTOd	22 16 14	125	x	-35
Ø34	RCL5	36 Ø5	Ø8Ø	*LBL4	21 Ø4	126	X ²	53
Ø35	1	Ø1	Ø81	RCL8	36 Ø8	127	+	-55
Ø36	Ø	ØØ	Ø82	RCL5	36 Ø5	128	√X	54
Ø37	x	-35	Ø83	X=Y?	16-33	129	RCL1	36 Ø1
Ø38	+	-55	Ø84	GTOc	22 16 13	13Ø	RCL3	36 Ø3
Ø39	PRTX	-14	Ø85	1	Ø1	131	x	-35
Ø4Ø	RTN	24	Ø86	+	-55	132	X≠Y	-41
Ø41	*LBLC	21 13	Ø87	STO5	35 Ø5	133	÷	-24
Ø42	RCL8	36 Ø8	Ø88	Ø	ØØ	134	RTN	24
Ø43	RCL7	36 Ø7	Ø89	STO6	35 Ø6	135	*LBL8	21 Ø8
Ø44	X>Y?	16-34	Ø9Ø	GTO7	22 Ø7	136	RCL4	36 Ø4
Ø45	R/S	51	Ø91	*LBLd	21 16 14	137	PRTX	-14
Ø46	Ø	ØØ	Ø92	RCLA	36 11	138	RCL5	36 Ø5

Card 1. Tetragonal (Concluded)

139	PRTX	-14	141	PRTX	-14	142	RTN	24
140	RCL6	36 06						

Card 2. Tetragonal

001	*LBLD	21 14	048	X>Y?	16-34	095	X>Y?	16-34
002	GSBe	23 16 15	049	GT07	22 07	096	GT08	22 08
003	÷	-24	050	X<0?	16-45	097	X<0?	16-45
004	GSB4	23 04	051	GT07	22 07	098	GT08	22 08
005	÷	-24	052	RCL7	36 07	099	9	09
006	+	-55	053	1	01	100	RCL5	36 05
007	STOA	35 11	054	0	00	101	X>Y?	16-34
008	GSB2	23 02	055	0	00	102	GT08	22 08
009	RCL1	36 01	056	x	-35	103	X<0?	16-45
010	X ²	53	057	+	-55	104	GT08	22 08
011	÷	-24	058	RCL8	36 08	105	9	09
012	RCL6	36 06	059	1	01	106	RCL6	36 06
013	RCL3	36 03	060	0	00	107	X>Y?	16-34
014	÷	-24	061	x	-35	108	GT08	22 08
015	GSB6	23 06	062	+	-55	109	X<0?	16-45
016	÷	-24	063	PRTX	-14	110	GT08	22 08
017	RCL9	36 09	064	RTN	24	111	RCL4	36 04
018	RCL3	36 03	065	*LBL	21 15	112	1	01
019	÷	-24	066	GSBe	23 16 15	113	0	00
020	*LBL9	21 09	067	x	-35	114	0	00
021	X ²	53	068	RCL6	36 06	115	x	-35
022	+	-55	069	RCL9	36 09	116	+	-55
023	x	-35	070	x	-35	117	RCL5	36 05
024	√X	54	071	RCL3	36 03	118	1	01
025	RCLA	36 11	072	X ²	53	119	0	00
026	X⇒Y	-41	073	x	-35	120	x	-35
027	÷	-24	074	+	-55	121	+	-55
028	COS ⁻¹	16 42	075	STOA	35 11	122	PRTX	-14
029	SPC	16-11	076	GSB2	23 02	123	RTN	24
030	FIX	-11	077	RCL1	36 01	124	*LBL2	21 02
031	DSP2	-63 02	078	X ²	53	125	RCL4	36 04
032	PRTX	-14	079	x	-35	126	X ²	53
033	GSB1	23 01	080	RCL6	36 06	127	RCL5	36 05
034	9	09	081	RCL3	36 03	128	X ²	53
035	RCL7	36 07	082	x	-35	129	+	-55
036	X>Y?	16-34	083	GSB6	23 06	130	RTN	24
037	GT07	22 07	084	x	-35	131	*LBL3	21 03
038	X<0?	16-45	085	RCL9	36 09	132	RCL7	36 07
039	GT07	22 07	086	RCL3	36 03	133	X ²	53
040	9	09	087	x	-35	134	RCL8	36 08
041	RCL8	36 08	088	GSB9	23 09	135	X ²	53
042	X>Y?	16-34	089	RTN	24	136	+	-55
043	GT07	22 07	090	*LBL1	21 01	137	RTN	24
044	X<0?	16-45	091	FIX	-11	138	*LBL4	21 04
045	GT07	22 07	092	DSP0	-63 00	139	RCL6	36 06
046	9	09	093	9	09	140	RCL9	36 09
047	RCL9	36 09	094	RCL4	36 04	141	x	-35

Card 2. Tetragonal (Concluded)

142	RCL3	36	Ø3	155	RCL8	36	Ø8	167	RTN		24
143	X ²		53	156	PRTX		-14	168	*LBL _e	21 16	15
144	RTN		24	157	RCL9	36	Ø9	169	RCL4		36 Ø4
145	*LBL6	21	Ø6	158	PRTX		-14	170	RCL7		36 Ø7
146	X ²		53	159	RTN		24	171	x		-35
147	+		-55	160	*LBL8	21	Ø8	172	RCL5		36 Ø5
148	GSB3	23	Ø3	161	RCL4	36	Ø4	173	RCL8		36 Ø8
149	RCL1	36	Ø1	162	PRTX		-14	174	x		-35
150	X ²		53	163	RCL5	36	Ø5	175	+		-55
151	RTN		24	164	PRTX		-14	176	RCL1	36	Ø1
152	*LBL7	21	Ø7	165	RCL6	36	Ø6	177	X ²		53
153	RCL7	36	Ø7	166	PRTX		-14	178	RTN		24
154	PRTX		-14								

Card 3. Tetragonal

ØØ1	*LBLB	21	12	Ø37	RCL6	36	Ø6	Ø73	R/S		51
ØØ2	Ø		ØØ	Ø38	X=Ø?		16-43	Ø74	GSBe	23 16	15
ØØ3	STOØ	35	ØØ	Ø39	GTO6		22 Ø6	Ø75	GTOa	22 16	11
ØØ4	STOC	35	13	Ø40	*LBL4	21	Ø4	Ø76	*LBL _e	21 16	15
ØØ5	*LBLa	21	16 11	Ø41	RCLA	36	11	Ø77	RCL4		36 Ø4
ØØ6	GSB2	23	Ø2	Ø42	X ²		53	Ø78	STO1		35 Ø1
ØØ7	RCL9	36	Ø9	Ø43	GSB2	23	Ø2	Ø79	RCL5		36 Ø5
ØØ8	X ²		53	Ø44	RCLD	36	14	Ø80	STO2		35 Ø2
ØØ9	x		-35	Ø45	X ²		53	Ø81	RCL6		36 Ø6
Ø10	GSB3	23	Ø3	Ø46	x		-35	Ø82	STO3		35 Ø3
Ø11	RCL6	36	Ø6	Ø47	-		-45	Ø83	RCL7		36 Ø7
Ø12	X ²		53	Ø48	X=Ø?		16-43	Ø84	STO4		35 Ø4
Ø13	x		-35	Ø49	GTO6	22	Ø6	Ø85	RCL8		36 Ø8
Ø14	-		-45	Ø50	1/X		52	Ø86	STO5		35 Ø5
Ø15	X=Ø?		16-43	Ø51	ABS	16	31	Ø87	RCL9		36 Ø9
Ø16	GTO9	22	Ø9	Ø52	√X		54	Ø88	STO6		35 Ø6
Ø17	RCL _E	36	15	Ø53	RCLA	36	11	Ø89	RCL1		36 Ø1
Ø18	RCL9	36	Ø9	Ø54	x		-35	Ø90	STO7		35 Ø7
Ø19	x		-35	Ø55	RCLD	36	14	Ø91	RCL2		36 Ø2
Ø20	X ²		53	Ø56	x		-35	Ø92	STO8		35 Ø8
Ø21	RCLD	36	14	Ø57	RCL6	36	Ø6	Ø93	RCL3		36 Ø3
Ø22	RCL6	36	Ø6	Ø58	x		-35	Ø94	STO9		35 Ø9
Ø23	x		-35	Ø59	FIX		-11	Ø95	RCLD		36 14
Ø24	X ²		53	Ø60	PRTX		-14	Ø96	STOØ		35 ØØ
Ø25	-		-45	Ø61	RTN		24	Ø97	RCL _E		36 15
Ø26	÷		-24	Ø62	*LBL6	21	Ø6	Ø98	STOD		35 14
Ø27	ABS	16	31	Ø63	RCLC	36	13	Ø99	RCLØ		36 ØØ
Ø28	√X		54	Ø64	X≠Ø?		16-42	100	STOE		35 15
Ø29	RCLD	36	14	Ø65	R/S		51	101	RTN		24
Ø30	x		-35	Ø66	GSBe	23 16	15	102	*LBL2	21	Ø2
Ø31	RCL _E	36	15	Ø67	1		Ø1	103	RCL4		36 Ø4
Ø32	x		-35	Ø68	STOC	35	13	104	X ²		53
Ø33	FIX		-11	Ø69	GTO4	22	Ø4	105	RCL5	36	Ø5
Ø34	DSP4	-63	Ø4	Ø70	*LBL9	21	Ø9	106	X ²		53
Ø35	PRTX		-14	Ø71	RCLØ	36	ØØ	107	+		-55
Ø36	STOA	35	11	Ø72	X≠Ø?		16-42	108	RTN		24

Card 3. Tetragonal (Concluded)

109	*LBL3	21 03	112	RCL8	36 08	115	RTN	24
110	RCL7	36 07	113	X ²	53	116	R/S	51
111	X ²	53	114	+	-55			

Program 4: Orthorhombic System Crystal Parameters

Program use- This program is used to calculate d spacings of crystal planes, interplanar angles (ϕ), interzonal angles (ρ), and cell edges for the orthorhombic crystal system. The applicable formulas are:

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

$$a^2 = \frac{d_1^2 d_2^2 d_3^4 [(h_3^2 l_2^2 - h_2^2 l_3^2)(k_1^2 l_3^2 - k_3^2 l_1^2) - (k_2^2 l_3^2 - k_3^2 l_2^2)(h_3^2 l_1^2 - h_1^2 l_3^2)]}{d_3^4 l_3^2 [d_2^2 (k_2^2 l_3^2 - k_3^2 l_2^2) - d_1^2 (k_1^2 l_3^2 - k_3^2 l_1^2)]}$$

$$+ d_1^2 d_2^2 d_3^2 [l_2^2 (k_1^2 l_3^2 - k_3^2 l_1^2) - l_1^2 (k_2^2 l_3^2 - k_3^2 l_2^2)]$$

$$b^2 = \frac{d_2^2 d_3^2 (k_2^2 l_3^2 - k_3^2 l_2^2)}{d_3^2 l_3^2 - d_2^2 l_2^2 + [d_2^2 d_3^2 (h_3^2 l_2^2 - h_2^2 l_3^2) / a^2]}$$

$$c^2 = \frac{d_3^2 l_3^2}{1 - (d_3^2 h_3^2 / a^2) - (d_3^2 k_3^2 / b^2)}$$

$$\cos \phi = \frac{h_1 h_2 / a^2 + k_1 k_2 / b^2 + l_1 l_2 / c^2}{[(h_1^2 / a^2 + k_1^2 / b^2 + l_1^2 / c^2)(h_2^2 / a^2 + k_2^2 / b^2 + l_2^2 / c^2)]^{1/2}}$$

$$\cos \rho = \frac{a^2 u_1 u_2 + b^2 v_1 v_2 + c^2 w_1 w_2}{[(a^2 u_1^2 + b^2 v_1^2 + c^2 w_1^2)(a^2 u_2^2 + b^2 v_2^2 + c^2 w_2^2)]^{1/2}}$$

The input and output parameters are:

	Input parameters	Output parameters ^a
Label A	Register 1- a	d or d
Card 1	Register 2- b	hk1
Calculate d	Register 3- c	k
	Register 4- h	l
	Register 5- k	
	Register 6- l	
Label B	Register 1- h ₁	a
Card 2	Register 2- k ₁	b
Calculate a,b,c	Register 3- l ₁	c
	Register 4- h ₂	
	Register 5- k ₂	
	Register 6- l ₂	

	Input parameters	Output parameters ^a	
	Register 7- h_3		
	Register 8- k_3		
	Register 9- l_3		
	Register A- d_1		
	Register B- d_2		
	Register C- d_3		
Label C	Register 1- a	d	
Card 1	Register 2- b	hkl	
Calculate all possible d's within limits	Register 3- c		
	Register 7- largest h to be printed		
	Register 8- largest k to be printed		
	Register 9- largest l to be printed		
	Register E- only d values larger than this printed		
Label D	Register 1- a	ϕ	or ϕ
Card 3	Register 2- b	$h_1k_1l_1$	h_1
Calculate angle (ϕ) between crystal planes	Register 3- c	$h_2k_2l_2$	k_1
	Register 4- h_1		l_1
	Register 5- k_1		h_2
	Register 6- l_1		k_2
	Register 7- h_2		l_2
	Register 8- k_2		
	Register 9- l_2		
Label E	Register 1- a	ρ	or ρ
Card 3	Register 2- b	$u_1v_1w_2$	u_1
Calculate angle (ρ) between crystal zones	Register 3- c	$u_2v_2w_2$	v_1
	Register 4- u_1		w_1
	Register 5- v_1		u_2
	Register 6- w_1		v_2
	Register 7- u_2		w_2
	Register 8- v_2		
	Register 9- w_2		

^aIf h, k, and l (u, v, and w) are 0 or positive and less than 10, output is in the form hkl or $u_1v_1w_1$ or $h_1k_1l_1$. If h, k, or l (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h & u \\ k & v \\ l & w \end{matrix}$ (vertical rather than horizontal format).

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push E for Label E). The actual program follows.

Card 1. Orthorhombic

001	*LBLA	21 11	049	STO5	35 05	097	+	-55
002	GSB1	23 01	050	STO6	35 06	098	STO4	36 04
003	*LBLa	21 16 11	051	STOA	35 11	099	0	00
004	SPC	16-11	052	*LBL0	21 00	100	STO5	35 05
005	PRTX	-14	053	RCL9	36 09	101	STO6	35 06
006	DSP0	-63 00	054	RCL6	36 06	102	1	01
007	9	09	055	X=Y?	16-33	103	STOB	35 12
008	RCL4	36 04	056	GTOb	22 16 12	104	GTO7	22 07
009	X>Y?	16-34	057	1	01	105	*LBL1	21 01
010	GTO9	22 09	058	+	-55	106	DSP4	-63 04
011	X<0?	16-45	059	STO6	35 06	107	RCL4	36 04
012	GTO9	22 09	060	0	00	108	RCL1	36 01
013	9	09	061	STOB	35 12	109	÷	-24
014	RCL5	36 05	062	*LBL7	21 07	110	X ²	53
015	X>Y?	16-34	063	0	00	111	RCL5	36 05
016	GTO9	22 09	064	STOA	35 11	112	RCL2	36 02
017	X<0?	16-45	065	GSB1	23 01	113	÷	-24
018	GTO9	22-09	066	RCL6	36 15	114	X ²	53
019	9	09	067	X>Y?	16-34	115	+	-55
020	RCL6	36 06	068	GTO3	22 03	116	RCL6	36 06
021	X>Y?	16-34	069	X≠Y	-41	117	RCL3	36 03
022	GTO9	22 09	070	GSBa	23 16 11	118	÷	-24
023	X<0?	16-45	071	GTO0	22 00	119	X ²	53
024	GTO9	22 09	072	*LBLb	21 16 12	120	+	-55
025	RCL4	36 04	073	RCL6	36 06	121	1/X	52
026	1	01	074	X=0?	16-43	122	√X	54
027	0	00	075	GTO4	22 04	123	RTN	24
028	0	00	076	*LBL5	21 05	124	*LBL3	21 03
029	x	-35	077	RCL8	36 08	125	1	01
030	+	-55	078	RCL5	36 05	126	STOA	35 11
031	RCL5	36 05	079	X=Y?	16-33	127	GTOb	22 16 12
032	1	01	080	GTOc	22 16 13	128	*LBL4	21 04
033	0	00	081	1	01	129	RCL9	36 09
034	x	-35	082	+	-55	130	X≠0?	16-42
035	+	-55	083	STO5	35 05	131	GTOc	22 16 13
036	PRTX	-14	084	0	00	132	RCLA	36 11
037	RTN	24	085	STO6	35 06	133	X≠0?	16-42
038	*LBL9	21 09	086	GTO7	22 07	134	GTOc	22 16 13
039	RCL4	36 04	087	*LBLc	21 16 13	135	GTO5	22 05
040	PRTX	-14	088	RCL5	36 05	136	*LBL6	21 06
041	RCL5	36 05	089	X=0?	16-43	137	RCL8	36 08
042	PRTX	-14	090	GTO6	22 06	138	X≠0?	16-42
043	RCL6	36 06	091	*LBL8	21 08	139	R/S	51
044	PRTX	-14	092	RCL7	36 07	140	RCLB	36 12
045	RTN	24	093	RCL4	36 04	141	X≠0?	16-42
046	*LBLC	21 13	094	X=Y?	16-33	142	R/S	51
047	0	00	095	R/S	51	143	GTO8	22 08
048	STO4	35 04	096	1	01			

Card 2. Orthorhombic

001	*LBLB	21 12	052	RCL0	36 00	103	+	-55
002	SPC	16-11	053	x	-35	104	X=0?	16-43
003	P=S	16-51	054	RCLE	36 15	105	GTOb	22 16 12
004	0	00	055	RCLI	36 46	106	RCLC	36 13
005	STO9	35 09	056	x	-35	107	RCL9	36 09
006	P=S	16-51	057	-	-45	108	GSB1	23 01
007	DSP4	-63 04	058	X=0?	16-43	109	X=0?	16-43
008	GSB4	23 04	059	GTO7	22 07	110	GTOb	22 16 12
009	*LBL8	21 08	060	X=Y	-41	111	X=Y	-41
010	RCL7	36 07	061	÷	-24	112	÷	-24
011	RCL3	36 03	062	STO0	35 00	113	ABS	16 31
012	GSB1	23 01	063	ABS	16 31	114	√X	54
013	RCL1	36 01	064	√X	54	115	PRTX	-14
014	RCL9	36 09	065	PRTX	-14	116	RTN	24
015	GSB2	23 02	066	*LBLe	21 16 15	117	*LBL1	21 01
016	RCLA	36 11	067	RCLD	36 14	118	x	-35
017	RCLC	36 13	068	RCL0	36 00	119	X ²	53
018	GSB3	23 03	069	÷	-24	120	RTN	24
019	STOI	35 46	070	RCLC	36 13	121	*LBL2	21 02
020	RCL2	36 02	071	RCL9	36 09	122	x	-35
021	RCL9	36 09	072	GSB1	23 01	123	X ²	53
022	GSB1	23 01	073	+	-55	124	-	-45
023	RCL8	36 08	074	RCLB	36 12	125	RTN	24
024	RCL3	36 03	075	RCL6	36 06	126	*LBL3	21 03
025	GSB2	23 02	076	GSB2	23 02	127	x	-35
026	RCLA	36 11	077	X=0?	16-43	128	X ²	53
027	RCLC	36 13	078	GTOa	22 16 11	129	x	-35
028	GSB3	23 03	079	RCLE	36 15	130	RTN	24
029	STO0	35 00	080	X=0?	16-43	131	*LBLa	21 16 11
030	RCLB	36 12	081	GTOa	22 16 11	132	GSBd	23 16 14
031	RCL6	36 06	082	X=Y	-41	133	GTOe	22 16 15
032	GSB1	23 01	083	÷	-24	134	*LBLb	21 16 12
033	RCL0	36 00	084	STOI	35 46	135	GSBd	23 16 14
034	x	-35	085	ABS	16 31	136	GTOc	22 16 13
035	RCLC	36 13	086	√X	54	137	*LBL7	21 07
036	RCL9	36 09	087	PRTX	-14	138	GSBd	23 16 14
037	GSB1	23 01	088	*LBLc	21 16 13	139	GTO8	22 08
038	RCLE	36 15	089	RCL7	36 07	140	*LBLd	21 16 14
039	RCL0	36 00	090	X ²	53	141	P=S	16-51
040	-	-45	091	RCL0	36 00	142	6	06
041	x	-35	092	÷	-24	143	RCL9	36 09
042	+	-55	093	RCL8	36 08	144	X=Y?	16-33
043	RCLA	36 11	094	X ²	53	145	R/S	51
044	RCL3	36 03	095	RCLI	36 46	146	1	01
045	GSB1	23 01	096	÷	-24	147	+	-55
046	RCLE	36 15	097	+	-55	148	STO9	35 09
047	x	-35	098	RCLC	36 13	149	P=S	16-51
048	-	-45	099	X ²	53	150	RCLA	36 11
049	X=0?	16-43	100	x	-35	151	RCL1	36 01
050	GTO7	22 07	101	CHS	-22	152	RCL2	36 02
051	RCLD	36 14	102	1	01	153	RCL3	36 03

Card 2. Orthorhombic (Concluded)

154	P=S	16-51	175	RCL5	36 05	196	RCL6	36 06
155	STO1	35 01	176	STO8	35 08	197	GSB1	23 01
156	R↓	-31	177	RCL6	36 06	198	RCL4	36 04
157	STO2	35 02	178	STO9	35 09	199	RCL9	36 09
158	R↓	-31	179	P=S	16-51	200	GSB2	23 02
159	STO3	35 03	180	RCL1	36 01	201	RCLB	36 12
160	R↓	-31	181	RCL2	36 02	202	RCLC	36 13
161	STO4	35 04	182	RCL3	36 03	203	GSB3	23 03
162	P=S	16-51	183	RCL4	36 04	204	STOD	35 14
163	RCLC	36 13	184	P=S	16-51	205	RCL5	36 05
164	STOA	35 11	185	STOB	35 12	206	RCL9	36 09
165	RCL7	36 07	186	R↓	-31	207	GSB1	23 01
166	STO1	35 01	187	STO4	35 04	208	RCL8	36 08
167	RCL8	36 08	188	R↓	-31	209	RCL6	36 06
168	STO2	35 02	189	STO5	35 05	210	GSB2	23 02
169	RCL9	36 09	190	R↓	-31	211	RCLB	36 12
170	STO3	35 03	191	STO6	35 06	212	RCLC	36 13
171	RCLB	36 12	192	GSB4	23 04	213	GSB3	23 03
172	STOC	35 13	193	RTN	24	214	STOE	35 15
173	RCL4	36 04	194	*LBL4	21 04	215	RTN	24
174	STO7	35 07	195	RCL7	36 07			

Card 3. Orthorhombic

001	*LBLD	21 14	029	RCL8	36 08	057	RCL5	36 05
002	GSB6	23 06	030	RCL2	36 02	058	X>Y?	16-34
003	÷	-24	031	÷	-24	059	GTO9	22 09
004	GSBd	23 16 14	032	X ²	53	060	X<0?	16-45
005	÷	-24	033	+	-55	061	GTO9	22 09
006	+	-55	034	RCL9	36 09	062	9	09
007	GSBe	23 16 15	035	RCL3	36 03	063	RCL6	36 06
008	÷	-24	036	÷	-24	064	X>Y?	16-34
009	+	-55	037	*LBL5	21 05	065	GTO9	22 09
010	STO0	35 00	038	X ²	53	066	X<0?	16-45
011	RCL4	36 04	039	+	-55	067	GTO9	22 09
012	RCL1	36 01	040	x	-35	068	RCL4	36 04
013	÷	-24	041	√X	54	069	1	01
014	X ²	53	042	RCL0	36 00	070	0	00
015	RCL5	36 05	043	X=Y	-41	071	0	00
016	RCL2	36 02	044	÷	-24	072	x	-35
017	÷	-24	045	COS ⁻¹	16 42	073	+	-55
018	X ²	53	046	DSP2	-63 02	074	RCL5	36 05
019	+	-55	047	SPC	16-11	075	1	01
020	RCL6	36 06	048	PRTX	-14	076	0	00
021	RCL3	36 03	049	DSP0	-63 00	077	x	-35
022	÷	-24	050	9	09	078	+	-55
023	X ²	53	051	RCL4	36 04	079	PRTX	-14
024	+	-55	052	X>Y?	16-34	080	*LBL4	21 04
025	RCL7	36 07	053	GTO9	22 09	081	9	09
026	RCL1	36 01	054	X<0?	16-45	082	RCL7	36 07
027	÷	-24	055	GTO9	22 09	083	X>Y?	16-34
028	X ²	53	056	9	09	084	GTO2	22 02

Card 3. Orthorhombic (Concluded)

085	X<0?	16-45	119	x	-35	153	RCL1	36	01
086	GTO2	22 02	120	+	-55	154	X ²		53
087	9	09	121	STO0	35 00	155	RTN		24
088	RCL8	36 08	122	RCL4	36 04	156	*LBLd	21 16	14
089	X>Y?	16-34	123	RCL1	36 01	157	RCL5	36	05
090	GTO2	22 02	124	x	-35	158	RCL8	36	08
091	X<0?	16-45	125	X ²	53	159	x		-35
092	GTO2	22 02	126	RCL5	36 05	160	RCL2	36	02
093	9	09	127	RCL2	36 02	161	X ²		53
094	RCL9	36 09	128	x	-35	162	RTN		24
095	X>Y?	16-34	129	X ²	53	163	*LBLe	21 16	15
096	GTO2	22 02	130	+	-55	164	RCL6	36	06
097	X<0?	16-45	131	RCL6	36 06	165	RCL9	36	09
098	GTO2	22 02	132	RCL3	36 03	166	x		-35
099	RCL7	36 07	133	x	-35	167	RCL3	36	03
100	1	01	134	X ²	53	168	X ²		53
101	0	00	135	+	-55	169	RTN		24
102	0	00	136	RCL7	36 07	170	*LBL2	21	02
103	x	-35	137	RCL1	36 01	171	RCL7	36	07
104	+	-55	138	x	-35	172	PRTX		-14
105	RCL8	36 08	139	X ²	53	173	RCL8	36	08
106	1	01	140	RCL8	36 08	174	PRTX		-14
107	0	00	141	RCL2	36 02	175	RCL9	36	09
108	x	-35	142	x	-35	176	PRTX		-14
109	+	-55	143	X ²	53	177	RTN		24
110	PRTX	-14	144	+	-55	178	*LBL9	21	09
111	RTN	24	145	RCL9	36 09	179	RCL4	36	04
112	*LBLE	21 15	146	RCL3	36 03	180	PRTX		-14
113	GSB6	23 06	147	x	-35	181	RCL5	36	05
114	x	-35	148	GTO5	22 05	182	PRTX		-14
115	GSBd	23 16 14	149	*LBL6	21 06	183	RCL6	36	06
116	x	-35	150	RCL4	36 04	184	PRTX		-14
117	+	-55	151	RCL7	36 07	185	GTO4	22	04
118	GSBe	23 16 15	152	x	-35	186	R/S		51

Program 5: Hexagonal System Crystal Parameters

Program use- This program is used to calculate d spacings of crystal planes, interplanar angles (ϕ), interzonal angles (ρ), and crystal axis lengths for the hexagonal crystal system. The applicable formulas are:

$$d = \frac{ac}{[(4/3)c^2(h^2 + hk + k^2) + a^2l^2]^{1/2}}$$

$$a = 2d_1d_2 \left[\frac{l_1^2(h_2^2 + h_2k_2 + k_2^2) - l_2^2(h_1^2 + h_1k_1 + k_1^2)}{3(l_1^2d_1^2 - l_2^2d_2^2)} \right]^{1/2}$$

$$c = l_1 d_1 \left[\frac{1}{1 - \{4d_1^2(h_1^2 + h_1 k_1 + k_1^2)/3a^2\}} \right]^{1/2}$$

$$\cos\phi = \frac{h_1 h_2 + k_1 k_2 + (1/2)(h_1 k_2 + k_1 h_2) + (3l_1 l_2 a^2/4c^2)}{\{[h_1^2 + k_1^2 + h_1 k_1 + (3a^2 l_1^2/4c^2)][h_2^2 + k_2^2 + h_2 k_2 + (3a^2 l_2^2/4c^2)]\}^{1/2}}$$

$$\cos\psi = \frac{u_1 u_2 + v_1 v_2 - (1/2)(u_1 v_2 + v_1 u_2) + (w_1 w_2 c^2/a^2)}{\{[u_1^2 + v_1^2 - u_1 v_1 + (c^2 w_1^2/a^2)][u_2^2 + v_2^2 - u_2 v_2 + (c^2 w_2^2/a^2)]\}^{1/2}}$$

The input and output parameters are:

	Input parameters	Output parameters ^a	
Label a	Register 1- a	d	or d
Card 1	Register 3- c	hkl	h
Calculate d	Register 4- h		k
	Register 5- k		l
	Register 6- l		
Label B	Register 4- h ₁	a	
Card 3	Register 5- k ₁	c	
Calculate a, c	Register 6- l ₁		
	Register 7- h ₂		
	Register 8- k ₂		
	Register 9- l ₂		
	Register D- d ₁		
	Register E- d ₂		
Label C	Register 1- a	d	
Card 1	Register 3- c	hkl	
Calculate all possible d's within limits	Register 7- largest h to be printed		
	Register 8- largest k to be printed		
NOTE: h < k	Register 9- largest l to be printed		
Reg. 7 < 8	Register E- only d values larger than this printed		
Label D	Register 1- a	φ	or φ
Card 2	Register 3- c	h ₁ k ₁ l ₁	h ₁
Calculate angle (φ) between crystal planes	Register 4- h ₁	h ₂ k ₂ l ₂	k ₁
	Register 5- k ₁		l ₁
	Register 6- l ₁		h ₂
	Register 7- h ₂		k ₂
	Register 8- k ₂		l ₂
	Register 9- l ₂		

	Input parameters	Output parameters ^a
Label E	Register 1- a	ρ or ρ
Card 2	Register 3- c	$u_1 v_1 w_1$ u_1
Calculate angle	Register 4- u_1	$u_2 v_2 w_2$ v_1
(ρ) between	Register 5- v_1	w_1
crystal zones	Register 6- w_1	u_2
	Register 7- u_2	v_2
	Register 8- v_2	w_2
	Register 9- w_2	

^aIf h, k, and l (u, v, and w) are 0 or positive and less than 10, output is in the form hkl (uvw). If h, k, or l (u, v, or w) are negative, or greater than 9, output is in the

form $\begin{matrix} h & u \\ k & v \\ l & w \end{matrix}$.

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push A for Label A). The actual program follows.

Card 1. Hexagonal									
001	*LBLA	21	11	030	+	-55	059	GSB0	23 00
002	GSB0	23	00	031	RCL5	36 05	060	RCL5	36 15
003	FIX	-11		032	1	01	061	X>Y?	16-34
004	PRTX	-14		033	0	00	062	GTO1	22 01
005	*LBLc	21	16 13	034	x	-35	063	X=Y	-41
006	DSP0	-63	00	035	+	-55	064	SPC	16-11
007	9	09		036	PRTX	-14	065	FIX	-11
008	RCL4	36	04	037	RTN	24	066	PRTX	-14
009	X>Y?	16-34		038	*LBLC	21 13	067	GSBc	23 16 13
010	GTOa	22	16 11	039	RCL8	36 08	068	GTO5	22 05
011	X<0?	16-45		040	RCL7	36 07	069	*LBL1	21 01
012	GTOa	22	16 11	041	X>Y?	16-34	070	1	01
013	9	09		042	R/S	51	071	STOA	35 11
014	RCL5	36	05	043	0	00	072	*LBL9	21 09
015	X>Y?	16-34		044	STOA	35 11	073	RCL6	36 06
016	GTOa	22	16 11	045	STO4	35 04	074	X=0?	16-43
017	X<0?	16-45		046	STO5	35 05	075	GTO2	22 02
018	GTOa	22	16 11	047	STO6	35 06	076	*LBL4	21 04
019	9	09		048	*LBL5	21 05	077	RCL8	36 08
020	RCL6	36	06	049	RCL9	36 09	078	RCL5	36 05
021	X>Y?	16-34		050	RCL6	36 06	079	X=Y?	16-33
022	GTOa	22	16 11	051	X=Y?	16-33	080	GTO8	22 08
023	X<0?	16-45		052	GTO9	22 09	081	1	01
024	GTOa	22	16 11	053	1	01	082	+	-55
025	RCL4	36	04	054	+	-55	083	STO5	35 05
026	1	01		055	STO6	35 06	084	0	00
027	0	00		056	*LBL6	21 06	085	STO6	35 06
028	0	00		057	0	00	086	GTO6	22 06
029	x	-35		058	STOA	35 11	087	*LBL2	21 02

Card 1. Hexagonal (Concluded)

088	RCLA	36 11	107	*LBL0	21 00	126	PRTX	-14
089	X=0?	16-43	108	GSBb	23 16 12	127	RCL5	36 05
090	GTO4	22 04	109	4	04	128	PRTX	-14
091	*LBL8	21 08	110	x	-35	129	RCL6	36 06
092	RCL5	36 05	111	3	03	130	PRTX	-14
093	RCL4	36 04	112	÷	-24	131	RTN	24
094	X=Y?	16-33	113	RCL1	36 01	132	*LBLb	21 16 12
095	R/S	51	114	X ²	53	133	DSP4	-63 04
096	RCL7	36 07	115	÷	-24	134	RCL4	36 04
097	X=Y?	16-33	116	RCL6	36 06	135	X ²	53
098	R/S	51	117	RCL3	36 03	136	RCL4	36 04
099	X⇒Y	-41	118	÷	-24	137	RCL5	36 05
100	1	01	119	X ²	53	138	x	-35
101	+	-55	120	+	-55	139	+	-55
102	STO4	35 04	121	1/X	52	140	RCL5	36 05
103	STO5	35 05	122	√X	54	141	X ²	53
104	0	00	123	RTN	24	142	+	-55
105	STO6	35 06	124	*LBLa	21 16 11	143	RTN	24
106	GTO6	22 06	125	RCL4	36 04			

Card 2. Hexagonal

001	*LBLD	21 14	031	x	-35	061	x	-35
002	GSB7	23 07	032	+	-55	062	RTN	24
003	RCL6	36 06	033	GSB9	23 09	063	*LBL2	21 02
004	RCL9	36 09	034	RCL3	36 03	064	x	-35
005	x	-35	035	RCL1	36 01	065	ABS	16 31
006	GSB8	23 08	036	÷	-24	066	√X	54
007	+	-55	037	RCL6	36 06	067	RCL0	36 00
008	GSB9	23 09	038	x	-35	068	X⇒Y	-41
009	RCL6	36 06	039	X ²	53	069	÷	-24
010	X ²	53	040	GSB0	23 00	070	COS ⁻¹	16 42
011	GSB8	23 08	041	-	-45	071	SPC	16-11
012	GSB0	23 00	042	RCL3	36 03	072	FIX	-11
013	+	-55	043	RCL1	36 01	073	DSP2	-63 02
014	RCL9	36 09	044	÷	-24	074	PRTX	-14
015	X ²	53	045	RCL9	36 09	075	*LBLa	21 16 11
016	GSB8	23 08	046	x	-35	076	FIX	-11
017	GSB6	23 06	047	X ²	53	077	DSP0	-63 00
018	+	-55	048	GSB6	23 06	078	9	09
019	GSB2	23 02	049	-	-45	079	RCL4	36 04
020	RTN	24	050	GSB2	23 02	080	X>Y?	16-34
021	*LBL E	21 15	051	RTN	24	081	GTOb	22 16 12
022	GSB7	23 07	052	*LBL6	21 06	082	X<0?	16-45
023	CHS	-22	053	RCL7	36 07	083	GTOb	22 16 12
024	RCL6	36 06	054	X ²	53	084	9	09
025	RCL9	36 09	055	+	-55	085	RCL5	36 05
026	x	-35	056	RCL8	36 08	086	X>Y?	16-34
027	RCL3	36 03	057	X ²	53	087	GTOb	22 16 12
028	RCL1	36 01	058	+	-55	088	X<0?	16-45
029	÷	-24	059	RCL7	36 07	089	GTOb	22 16 12
030	X ²	53	060	RCL8	36 08	090	9	09

Card 2. Hexagonal (Concluded)

091	RCL6	36 06	128	GTOd	22 16 14	165	2	02
092	X>Y?	16-34	129	9	09	166	÷	-24
093	GTOb	22 16 12	130	RCL9	36 09	167	RTN	24
094	X<0?	16-45	131	X>Y?	16-34	168	*LBL8	21 08
095	GTOb	22 16 12	132	GTOd	22 16 14	169	RCL1	36 01
096	RCL4	36 04	133	X<0?	16-45	170	RCL3	36 03
097	1	01	134	GTOd	22 16 14	171	÷	-24
098	0	00	135	RCL7	36 07	172	X ²	53
099	0	00	136	1	01	173	x	-35
100	x	-35	137	0	00	174	3	03
101	+	-55	138	0	00	175	x	-35
102	RCL5	36 05	139	x	-35	176	4	04
103	1	01	140	+	-55	177	÷	-24
104	0	00	141	RCL8	36 08	178	RTN	24
105	x	-35	142	1	01	179	*LBL9	21 09
106	+	-55	143	0	00	180	RCL5	36 05
107	PRTX	-14	144	x	-35	181	RCL8	36 08
108	GTOc	22 16 13	145	+	-55	182	x	-35
109	*LBLb	21 16 12	146	PRTX	-14	183	+	-55
110	RCL4	36 04	147	RTN	24	184	RCL4	36 04
111	PRTX	-14	148	*LBLd	21 16 14	185	RCL7	36 07
112	RCL5	36 05	149	RCL7	36 07	186	x	-35
113	PRTX	-14	150	PRTX	-14	187	+	-55
114	RCL6	36 06	151	RCL8	36 08	188	STO0	35 00
115	PRTX	-14	152	PRTX	-14	189	RTN	24
116	*LBLc	21 16 13	153	RCL9	36 09	190	*LBL0	21 00
117	9	09	154	PRTX	-14	191	RCL4	36 04
118	RCL7	36 07	155	RTN	24	192	X ²	53
119	X>Y?	16-34	156	*LBL7	21 07	193	+	-55
120	GTOd	22 16 14	157	DSP4	-63 04	194	RCL5	36 05
121	X<0?	16-45	158	RCL4	36 04	195	X ²	53
122	GTOd	22 16 14	159	RCL8	36 08	196	+	-55
123	9	09	160	x	-35	197	RCL4	36 04
124	RCL8	36 08	161	RCL5	36 05	198	RCL5	36 05
125	X>Y?	16-34	162	RCL7	36 07	199	x	-35
126	GTOd	22 16 14	163	x	-35	200	RTN	24
127	X<0?	16-45	164	+	-55			

Card 3. Hexagonal

001	*LBLB	21 12	013	X ²	53	025	RCL6	36 06
002	0	00	014	+	-55	026	RCLD	36 14
003	STOA	35 11	015	RCL6	36 06	027	x	-35
004	STOC	35 13	016	X ²	53	028	X ²	53
005	*LBL8	21 08	017	x	-35	029	RCL9	36 09
006	RCL7	36 07	018	GSBb	23 16 12	030	RCL E	36 15
007	X ²	53	019	RCL9	36 09	031	x	-35
008	RCL7	36 07	020	X ²	53	032	X ²	53
009	RCL8	36 08	021	x	-35	033	-	-45
010	x	-35	022	-	-45	034	3	03
011	+	-55	023	X=0?	16-43	035	x	-35
012	RCL8	36 08	024	GTO6	22 06	036	÷	-24

Card 3. Hexagonal (Concluded)

037	ABS	16 31	069	GTO7	22 07	101	RCL8	36 08
038	√X	54	070	1/X	52	102	STO5	35 05
039	2	02	071	ABS	16 31	103	RCL9	36 09
040	x	-35	072	√X	54	104	STO6	35 06
041	RCLD	36 14	073	RCL6	36 06	105	RCL1	36 01
042	x	-35	074	x	-35	106	STO7	35 07
043	RCLC	36 15	075	RCLD	36 14	107	RCL2	36 02
044	x	-35	076	x	-35	108	STO8	35 08
045	STO0	35 00	077	FIX	-11	109	RCL3	36 03
046	SPC	16-11	078	PRTX	-14	110	STO9	35 09
047	FIX	-11	079	RTN	24	111	RCLD	36 14
048	DSP4	-63 04	080	*LBLb	21 16 12	112	STOA	35 11
049	PRTX	-14	081	DSP4	-63 04	113	RCLC	36 15
050	*LBL9	21 09	082	RCL4	36 04	114	STOD	35 14
051	RCL6	36 06	083	X ²	53	115	RCLA	36 11
052	x=0?	16-43	084	RCL4	36 04	116	STOE	35 15
053	GTO7	22 07	085	RCL5	36 05	117	RTN	24
054	GSBb	23 16 12	086	x	-35	118	*LBL6	21 06
055	RCLD	36 14	087	+	-55	119	RCLA	36 11
056	X ²	53	088	RCL5	36 05	120	X≠0?	16-42
057	x	-35	089	X ²	53	121	R/S	51
058	4	04	090	+	-55	122	GSBe	23 16 15
059	x	-35	091	RTN	24	123	GTO8	22 08
060	3	03	092	*LBLc	21 16 15	124	*LBL7	21 07
061	÷	-24	093	RCL4	36 04	125	RCLC	36 13
062	RCL0	36 00	094	STO1	35 01	126	X≠0?	16-42
063	X ²	53	095	RCL5	36 05	127	R/S	51
064	÷	-24	096	STO2	35 02	128	GSBe	23 16 15
065	CHS	-22	097	RCL6	36 06	129	1	01
066	1	01	098	STO3	35 03	130	STOC	35 13
067	+	-55	099	RCL7	36 07	131	GTO9	22 09
068	X=0?	16-43	100	STO4	35 04	132	R/S	51

Program 6: Rhombohedral System Crystal Parameters

Program use- This program is used to calculate d spacings of crystal planes, interplanar angles, interzonal angles, crystal axis length, and axial angle for the rhombohedral crystal system. The applicable formulas are:

$$\frac{1}{d^2} = \frac{(1 + \cos\alpha)\{(h^2 + k^2 + l^2) - (1 - \tan^2[\alpha/2])(hk + kl + lh)\}}{a^2(1 + \cos\alpha - 2 \cos^2\alpha)}$$

$$a^2 = \frac{d^2[(h^2 + k^2 + l^2)(1 + \cos\alpha) - 2(hk + kl + lh)\cos\alpha]}{1 + \cos\alpha - 2 \cos^2\alpha}$$

$$\cos\alpha = \frac{d_2^2(h_2^2 + k_2^2 + l_2^2) - d_1^2(h_1^2 + k_1^2 + l_1^2)}{d_1^2(h_1^2 + k_1^2 + l_1^2) - d_2^2(h_2^2 + k_2^2 + l_2^2) + 2d_2^2(h_2k_2 + k_2l_2 + l_2h_2) - 2d_1^2(h_1k_1 + k_1l_1 + l_1h_1)}$$

$$\cos\phi = \frac{H_1H_2 + K_1K_2 + (1/2)(H_1K_2 + K_1H_2) + L_1L_2\sin^2(\alpha/2)/(3 - 4\sin^2(\alpha/2))}{\left(\left[\left(H_1^2 + K_1^2 + H_1K_1 + \{L_1^2\sin^2(\alpha/2)/[3 - 4\sin^2(\alpha/2)]\} \right) \times \left(H_2^2 + K_2^2 + H_2K_2 + \{L_2^2\sin^2(\alpha/2)/[3 - 4\sin^2(\alpha/2)]\} \right) \right]^{1/2}}$$

where

$$H_1 = h_1 - l_1 \quad K_1 = k_1 - h_1 \quad L_1 = h_1 + k_1 + l_1$$

$$H_2 = h_2 - l_2 \quad K_2 = k_2 - h_2 \quad L_2 = h_2 + k_2 + l_2$$

and

$$\cos\phi = \frac{U_1U_2 + V_1V_2 - (1/2)(U_1V_2 + V_1U_2) + W_1W_2(9 - 12\sin^2(\alpha/2)/4\sin^2(\alpha/2))}{\left(\left[\left(U_1^2 + V_1^2 - U_1V_1 + \{W_1^2[9 - 12\sin^2(\alpha/2)]/4\sin^2(\alpha/2)\} \right) \times \left(U_2^2 + V_2^2 - U_2V_2 + \{W_2^2[9 - 12\sin^2(\alpha/2)]/4\sin^2(\alpha/2)\} \right) \right]^{1/2}}$$

where

$$U_1 = u_1 - w_1 \quad V_1 = v_1 - u_1 \quad W_1 = u_1 + v_1 + w_1$$

$$U_2 = u_2 - w_2 \quad V_2 = v_2 - u_2 \quad W_2 = u_2 + v_2 + w_2$$

The input and output parameters are:

	Input parameters	Output parameters ^a
Label A	Register 1- a	d or d
Card 1	Register 4- h	hkl
Calculate d	Register 5- k	k
	Register 6- l	l
	Register A- α	
Label B	Register 4- h ₁	a
Card 3	Register 5- k ₁	α
Calculate a, α	Register 6- l ₁	
	Register 7- h ₂	
	Register 8- k ₂	
	Register 9- l ₂	

	Input parameters	<u>Output parameters^a</u>		
	Register D- d_1			
	Register E- d_2			
Label C	Register 1- a	d	or	d
Card 1	Register 7- largest h	$hk1$		h
Calculate all possible d 's within limits	to be printed			k
	Register 8- largest k			1
	to be printed			
	Register 9- largest l			
	to be printed			
NOTE: $h < k < l$	Register A- α			
Reg. $7 < 8 < 9$	Register E- only d values larger than this printed			
Label D	Register 1- a	ϕ	or	ϕ
Card 2	Register 4- h_1	$h_1 k_1 l_1$		h_1
Calculate angle (ϕ) between crystal planes	Register 5- k_1	h_2		k_1
	Register 6- l_1	k_2		l_1
	Register 7- h_2	l_2		h_2
	Register 8- k_2			k_2
	Register 9- l_2			l_2
	Register A- α			
Label E	Register 1- a	ρ	or	ρ
Card 2	Register 4- u_1	$u_1 v_1 w_1$		u_1
Calculate angle (ρ) between crystal zones	Register 5- v_1	u_2		v_1
	Register 6- w_1	v_2		w_1
	Register 7- u_2	w_2		u_2
	Register 8- v_2			v_2
	Register 9- w_2			w_2
	Register A- α			

^aIf h , k , and l (u , v , and w) are 0, or positive and less than 10, output is in the form $hk1$ (uvw). If h , k , or l (u , v , or w) are negative, or greater than 9, output is in the form $\begin{matrix} h & u \\ k & v \\ l & w \end{matrix}$.

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push C for Label C). The actual program follows.

Card 1. Rhombohedral									
001	*LBLA	21	11	006	PRTX	-14	011	GTOb	22 16 12
002	GSB1	23	01	007	DSP0	-63 00	012	X<0?	16-45
003	*LBLa	21	16 11	008	9	09	013	GTOb	22 16 12
004	SPC	16-11		009	RCL4	36 04	014	9	09
005	DSP4	-63 04		010	X>Y?	16-34	015	RCL5	36 05

Card 1. Rhombohedral (Continued)

Ø16	X>Y?	16-34	Ø67	RCL5	36 Ø5	118	CHS	-22
Ø17	GTOb	22 16 12	Ø68	+	-55	119	STO4	35 Ø4
Ø18	X<Ø?	16-45	Ø69	X=Ø?	16-43	120	GTOØ	22 ØØ
Ø19	GTOb	22 16 12	Ø70	GTOØ	22 ØØ	121	*LBLc	21 16 13
Ø20	9	Ø9	Ø71	RCL6	36 Ø6	122	RCL8	36 Ø8
Ø21	RCL6	36 Ø6	Ø72	CHS	-22	123	RCL5	36 Ø5
Ø22	X>Y?	16-34	Ø73	STO6	35 Ø6	124	X=Y?	16-33
Ø23	GTOb	22 16 12	Ø74	GSB1	23 Ø1	125	GTOd	22 16 14
Ø24	X<Ø?	16-45	Ø75	RCLE	36 15	126	1	Ø1
Ø25	GTOb	22 16 12	Ø76	X>Y?	16-34	127	+	-55
Ø26	RCL4	36 Ø4	Ø77	GTO3	22 Ø3	128	STO5	35 Ø5
Ø27	1	Ø1	Ø78	X=Ø?	-41	129	STO6	35 Ø6
Ø28	Ø	ØØ	Ø79	GSBa	23 16 11	130	GTO7	22 Ø7
Ø29	Ø	ØØ	Ø80	*LBL3	21 Ø3	131	*LBLd	21 16 14
Ø30	x	-35	Ø81	RCL6	36 Ø6	132	RCL7	36 Ø7
Ø31	+	-55	Ø82	CHS	-22	133	RCL4	36 Ø4
Ø32	RCL5	36 Ø5	Ø83	STO6	35 Ø6	134	X=Y?	16-33
Ø33	1	Ø1	Ø84	RCL4	36 Ø4	135	R/S	51
Ø34	Ø	ØØ	Ø85	X=Ø?	16-43	136	1	Ø1
Ø35	x	-35	Ø86	GTOØ	22 ØØ	137	+	-55
Ø36	+	-55	Ø87	RCL6	36 Ø6	138	STO4	35 Ø4
Ø37	PRTX	-14	Ø88	RCL5	36 Ø5	139	STO5	35 Ø5
Ø38	RTN	24	Ø89	X=Y?	16-33	140	STO6	35 Ø6
Ø39	*LBLC	21 13	Ø90	GTO9	22 Ø9	141	GTO7	22 Ø7
Ø40	RCL9	36 Ø9	Ø91	CHS	-22	142	*LBLb	21 16 12
Ø41	RCL8	36 Ø8	Ø92	STO5	35 Ø5	143	RCL4	36 Ø4
Ø42	X>Y?	16-34	Ø93	GSB1	23 Ø1	144	PRTX	-14
Ø43	R/S	51	Ø94	RCLE	36 15	145	RCL5	36 Ø5
Ø44	RCL7	36 Ø7	Ø95	X>Y?	16-34	146	PRTX	-14
Ø45	X>Y?	16-34	Ø96	GTO4	22 Ø4	147	RCL6	36 Ø6
Ø46	R/S	51	Ø97	X=Ø?	-41	148	PRTX	-14
Ø47	Ø	ØØ	Ø98	GSBa	23 16 11	149	RTN	24
Ø48	STO4	35 Ø4	Ø99	*LBL4	21 Ø4	150	*LBL1	21 Ø1
Ø49	STO5	35 Ø5	100	RCL5	36 Ø5	151	RCL4	36 Ø4
Ø50	STO6	35 Ø6	101	CHS	-22	152	X ²	53
Ø51	*LBLØ	21 ØØ	102	STO5	35 Ø5	153	RCL5	36 Ø5
Ø52	RCL9	36 Ø9	103	*LBL9	21 Ø9	154	X ²	53
Ø53	RCL6	36 Ø6	104	RCL5	36 Ø5	155	+	-55
Ø54	X=Y?	16-33	105	RCL4	36 Ø4	156	RCL6	36 Ø6
Ø55	GTOc	22 16 13	106	X=Y?	16-33	157	X ²	53
Ø56	1	Ø1	107	GTOØ	22 ØØ	158	+	-55
Ø57	ST+6	35-55 Ø6	108	CHS	-22	159	RCL4	36 Ø4
Ø58	*LBL7	21 Ø7	109	STO4	35 Ø4	160	RCL5	36 Ø5
Ø59	GSB1	23 Ø1	110	GSB1	23 Ø1	161	x	-35
Ø60	RCLE	36 15	111	RCLE	36 15	162	RCL5	36 Ø5
Ø61	X>Y?	16-34	112	X>Y?	16-34	163	RCL6	36 Ø6
Ø62	GTO2	22 Ø2	113	GTO5	22 Ø5	164	x	-35
Ø63	X=Ø?	-41	114	X=Ø?	-41	165	+	-55
Ø64	GSBa	23 16 11	115	GSBa	23 16 11	166	RCL6	36 Ø6
Ø65	*LBL2	21 Ø2	116	*LBL5	21 Ø5	167	RCL4	36 Ø4
Ø66	RCL4	36 Ø4	117	RCL4	36 Ø4	168	x	-35

Card 1. Rhombohedral (Concluded)

169	+	-55	181	COS	42	192	RCLA	36 11
170	RCLA	36 11	182	1	01	193	COS	42
171	2	02	183	+	-55	194	X ²	53
172	÷	-24	184	x	-35	195	2	02
173	TAN	43	185	RCL1	36 01	196	x	-35
174	X ²	53	186	X ²	53	197	-	-45
175	CHS	-22	187	÷	-24	198	÷	-24
176	1	01	188	RCLA	36 11	199	1/X	52
177	+	-55	189	COS	42	200	ABS	16 31
178	x	-35	190	1	01	201	√X	54
179	-	-45	191	+	-55	202	RTN	24
180	RCLA	36 11						

Card 2. Rhombohedral

001	*LBLD	21 14	038	X ²	53	075	X>Y?	16-34
002	GSBB	23 12	039	GSB0	23 00	076	GTOa	22 16 11
003	RCLD	36 14	040	-	-45	077	X<0?	16-45
004	RCLI	36 46	041	RCL3	36 03	078	GTOa	22 16 11
005	x	-35	042	RCL2	36 02	079	9	09
006	GSB8	23 08	043	÷	-24	080	RCL6	36 06
007	+	-55	044	RCLI	36 46	081	X>Y?	16-34
008	GSB9	23 09	045	x	-35	082	GTOa	22 16 11
009	RCLD	36 14	046	X ²	53	083	X<0?	16-45
010	X ²	53	047	GSB6	23 06	084	GTOa	22 16 11
011	GSB8	23 08	048	-	-45	085	RCL4	36 04
012	GSB0	23 00	049	*LBL2	21 02	086	1	01
013	+	-55	050	x	-35	087	0	00
014	RCLI	36 46	051	ABS	16 31	088	0	00
015	X ²	53	052	√X	54	089	GSB7	23 07
016	GSB8	23 08	053	P⇒S	16-51	090	RCL5	36 05
017	GSB6	23 06	054	RCL0	36 00	091	1	01
018	+	-55	055	P⇒S	16-51	092	0	00
019	GSB2	23 02	056	X⇒Y	-41	093	GSB7	23 07
020	RTN	24	057	÷	-24	094	PRTX	-14
021	*LBL E	21 15	058	COS ⁻¹	16 42	095	GTOb	22 16 12
022	GSBB	23 12	059	SPC	16-11	096	*LBLa	21 16 11
023	CHS	-22	060	9	09	097	RCL4	36 04
024	RCLD	36 14	061	0	00	098	PRTX	-14
025	RCLI	36 46	062	X⇒Y	-41	099	RCL5	36 05
026	x	-35	063	X>Y?	16-34	100	PRTX	-14
027	RCL3	36 03	064	GSB5	23 05	101	RCL6	36 06
028	RCL2	36 02	065	DSP2	-63 02	102	PRTX	-14
029	÷	-24	066	PRTX	-14	103	*LBLb	21 16 12
030	X ²	53	067	9	09	104	RCL7	36 07
031	GSB7	23 07	068	RCL4	36 04	105	PRTX	-14
032	GSB9	23 09	069	X>Y?	16-34	106	RCL8	36 08
033	RCL3	36 03	070	GTOa	22 16 11	107	PRTX	-14
034	RCL2	36 02	071	X<0?	16-45	108	RCL9	36 09
035	÷	-24	072	GTOa	22 16 11	109	PRTX	-14
036	RCLD	36 14	073	9	09	110	RTN	24
037	x	-35	074	RCL5	36 05	111	*LBL6	21 06

Card 2. Rhombohedral (Concluded)

112	RCLE	36 15	150	+	-55	188	STOC	35 13
113	X ²	53	151	RCLB	36 12	189	RCL8	36 08
114	+	-55	152	RCLC	36 13	190	RCL7	36 07
115	RCL0	36 00	153	x	-35	191	-	-45
116	X ²	53	154	RTN	24	192	STO0	35 00
117	+	-55	155	*LBLB	21 12	193	RCL4	36 04
118	RCLE	36 15	156	RCLA	36 11	194	RCL5	36 05
119	RCL0	36 00	157	2	02	195	+	-55
120	x	-35	158	÷	-24	196	RCL6	36 06
121	RTN	24	159	SIN	41	197	+	-55
122	*LBL8	21 08	160	RCL1	36 01	198	STOD	35 14
123	RCL2	36 02	161	x	-35	199	RCL7	36 07
124	RCL3	36 03	162	2	02	200	RCL8	36 08
125	÷	-24	163	x	-35	201	+	-55
126	X ²	53	164	STO2	35 02	202	RCL9	36 09
127	x	-35	165	RCL1	36 01	203	+	-55
128	3	03	166	X ²	53	204	STOI	35 46
129	x	-35	167	9	09	205	RCLB	36 12
130	4	04	168	x	-35	206	RCL0	36 00
131	÷	-24	169	RCL2	36 02	207	x	-35
132	RTN	24	170	X ²	53	208	RCLC	36 13
133	*LBL9	21 09	171	3	03	209	RCLE	36 15
134	RCLC	36 13	172	x	-35	210	GSB7	23 07
135	RCL0	36 00	173	-	-45	211	2	02
136	GSB7	23 07	174	ABS	16 31	212	÷	-24
137	RCLB	36 12	175	√X	54	213	RTN	24
138	RCLE	36 15	176	STO3	35 03	214	*LBL5	21 05
139	GSB7	23 07	177	RCL4	36 04	215	1	01
140	P=S	16-51	178	RCL6	36 06	216	8	08
141	STO0	35 00	179	-	-45	217	0	00
142	P=S	16-51	180	STOB	35 12	218	X=Y	-41
143	RTN	24	181	RCL7	36 07	219	-	-45
144	*LBL0	21 00	182	RCL9	36 09	220	RTN	24
145	RCLB	36 12	183	-	-45	221	*LBL7	21 07
146	X ²	53	184	STOE	35 15	222	x	-35
147	+	-55	185	RCL5	36 05	223	+	-55
148	RCLC	36 13	186	RCL4	36 04	224	RTN	24
149	X ²	53	187	-	-45			

Card 3. Rhombohedral

001	*LBLB	21 12	012	RCL5	36 05	023	RCL7	36 07
002	RCL4	36 04	013	x	-35	024	X ²	53
003	X ²	53	014	RCL5	36 05	025	RCL8	36 08
004	RCL5	36 05	015	RCL6	36 06	026	X ²	53
005	X ²	53	016	x	-35	027	+	-55
006	+	-55	017	+	-55	028	RCL9	36 09
007	RCL6	36 06	018	RCL6	36 06	029	X ²	53
008	X ²	53	019	RCL4	36 04	030	+	-55
009	+	-55	020	x	-35	031	STO2	35 02
010	STO0	35 00	021	+	-55	032	RCL7	36 07
011	RCL4	36 04	022	STO1	35 01	033	RCL8	36 08

Card 3. Rhombohedral (Concluded)

034	x	-35	071	9	09	107	ABS	16	31
035	RCL8	36 08	072	0	00	108	√X		54
036	RCL9	36 09	073	X=Y	-41	109	SPC	16	-11
037	x	-35	074	X>Y?	16-34	110	FIX		-11
038	+	-55	075	GSB1	23 01	111	DSP4	-63	04
039	RCL9	36 09	076	STOA	35 11	112	PRTX		-14
040	RCL7	36 07	077	RCL0	36 00	113	RCLA	36	11
041	x	-35	078	RCLA	36 11	114	DSP2	-63	02
042	+	-55	079	COS	42	115	PRTX		-14
043	STO3	35 03	080	x	-35	116	RTN		24
044	RCL5	36 15	081	RCL0	36 00	117	*LBL1	21	01
045	X ²	53	082	+	-55	118	1		01
046	RCL2	36 02	083	RCL1	36 01	119	8		08
047	x	-35	084	RCLA	36 11	120	0		00
048	RCLD	36 14	085	COS	42	121	X=Y		-41
049	X ²	53	086	x	-35	122	-		-45
050	RCL0	36 00	087	2	02	123	RTN		24
051	x	-35	088	x	-35	124	*LBLa	21	16 11
052	-	-45	089	-	-45	125	RCL2	36	02
053	STOB	35 12	090	RCLD	36 14	126	RCLA	36	11
054	CHS	-22	091	X ²	53	127	COS		42
055	RCL5	36 15	092	x	-35	128	x		-35
056	X ²	53	093	X=0?	16-43	129	RCL2	36	02
057	RCL3	36 03	094	GTOa	22 16 11	130	+		-55
058	x	-35	095	*LBL2	21 02	131	RCL3	36	03
059	RCLD	36 14	096	RCLA	36 11	132	RCLA	36	11
060	X ²	53	097	COS	42	133	COS		42
061	RCL1	36 01	098	1	01	134	x		-35
062	x	-35	099	+	-55	135	2		02
063	-	-45	100	RCLA	36 11	136	x		-35
064	2	02	101	COS	42	137	-		-45
065	x	-35	102	X ²	53	138	RCL5	36	15
066	+	-55	103	2	02	139	X ²		53
067	RCLB	36 12	104	x	-35	140	x		-35
068	X=Y	-41	105	-	-45	141	GTO2	22	02
069	÷	-24	106	÷	-24	142	R/S		51
070	COS ⁻¹	16 42							

Program 7: Rhombohedral ⇌ Hexagonal Conversions

Program use- This program is used to change from rhombohedral crystal parameters to hexagonal crystal parameters, and vice versa. Crystal indices, axis lengths, and axial angle can be calculated from one system to the other.

In some instances it may be of use to convert crystal parameters from the rhombohedral crystal system to the hexagonal crystal system, or vice versa. This program converts crystal indices (hkl or hkil) and lattice constants ($a_H c_H$ or $a_R \alpha_R$) from one system to the other.

The applicable formulas are:

$$a_H = 2a_R \sin \frac{\alpha_R}{2}$$

$$c_H = (9a_R^2 - 3a_H^2)^{1/2}$$

$$h_H = h_R - l_R$$

$$k_H = k_R - h_R$$

$$i_H = -(h_H + k_H)$$

$$l_H = h_R + k_R + l_R$$

$$a_R = \left(\frac{a_H^2}{3} + \frac{c_H^2}{9} \right)^{1/2}$$

$$\sin \frac{\alpha_R}{2} = \frac{3}{2} \left(3 + \frac{c_H^2}{a_H^2} \right)^{1/2}$$

$$h_R = \frac{h_H - k_H + l_H}{3}$$

$$k_R = \frac{h_H + 2k_H + l_H}{3}$$

$$l_R = \frac{-2h_H - k_H + l_H}{3}$$

The input and output parameters are:

	Input parameters	Output parameters
Label A	Register 1- a_R	a_H
Calculate a_H, c_H	Register A- α_R	c_H
Label B ^a	Register 4- h_R	$h_H k_H \cdot l_H$ or h_H
Calculate	Register 5- k_R	k_H
$h_H k_H \cdot l_H$	Register 6- l_R	l_H
Label C	Register 1- a_H	a_R
Calculate a_R, α_R	Register 3- c_H	α_R
Label D ^a	Register 4- h_H	$h_R k_R l_R$ or h_R
Calculate	Register 5- k_H	k_R
$h_R k_R l_R$	Register 6- l_H	l_R

	Input parameters	Output parameters
Label E	Register 4- h_R	h_H
Calculate	Register 5- k_R	k_H
$h_H k_H i_H l_H$	Register 6- l_R	i_H l_H

^aIf h, k, and l are 0, or positive integers less than 10, output is in the form hkl or hk.l. If h, k, or l are negative, greater than 9, or not integers,

output is in the form $\begin{matrix} h \\ k \\ l \end{matrix}$.

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push B for Label B). The actual program follows.

Hexagonal \rightleftharpoons Rhombohedral Calculations

001	*LBLA	21 11	034	X<0?	16-45	067	PRTX	-14
002	RCLA	36 11	035	GTOa	22 16 11	068	RCLD	36 14
003	2	02	036	9	09	069	PRTX	-14
004	÷	-24	037	RCLC	36 13	070	RTN	24
005	SIN	41	038	X>Y?	16-34	071	*LBLC	21 13
006	RCL1	36 01	039	GTOa	22 16 11	072	RCL1	36 01
007	x	-35	040	X<0?	16-45	073	X ²	53
008	2	02	041	GTOa	22 16 11	074	3	03
009	x	-35	042	9	09	075	÷	-24
010	SPC	16-11	043	RCLD	36 14	076	RCL3	36 03
011	DSP4	-63 04	044	X>Y?	16-34	077	X ²	53
012	PRTX	-14	045	GTOa	22 16 11	078	9	09
013	STO0	35 00	046	X<0?	16-45	079	÷	-24
014	RCL1	36 01	047	GTOa	22 16 11	080	+	-55
015	X ²	53	048	DSP1	-63 01	081	√X	54
016	9	09	049	RCLB	36 12	082	SPC	16-11
017	x	-35	050	1	01	083	DSP4	-63 04
018	RCL0	36 00	051	0	00	084	PRTX	-14
019	X ²	53	052	x	-35	085	RCL3	36 03
020	3	03	053	RCLC	36 13	086	RCL1	36 01
021	x	-35	054	+	-55	087	÷	-24
022	-	-45	055	RCLD	36 14	088	X ²	53
023	ABS	16 31	056	1	01	089	3	03
024	√X	54	057	0	00	090	+	-55
025	PRTX	-14	058	÷	-24	091	√X	54
026	RTN	24	059	+	-55	092	2	02
027	*LBLB	21 12	060	PRTX	-14	093	x	-35
028	GSB2	23 02	061	RTN	24	094	3	03
029	SPC	16-11	062	*LBLa	21 16 11	095	X=Y	-41
030	9	09	063	DSP0	-63 00	096	÷	-24
031	RCLB	36 12	064	RCLB	36 12	097	SIN ⁻¹	16-41
032	X>Y?	16-34	065	PRTX	-14	098	2	02
033	GTOa	22 16 11	066	RCLC	36 13	099	x	-35

Hexagonal \rightleftharpoons Rhombohedral Calculations (Concluded)

100	DSP2	-63 02	137	GTOa	22 16 11	174	PRTX	-14
101	PRTX	-14	138	X<0?	16-45	175	RTN	24
102	RTN	24	139	GTOa	22 16 11	176	*LBLE	21 15
103	*LBLD	21 14	140	FRC	16 44	177	GSB2	23 02
104	RCL4	36 04	141	X#0?	16-42	178	RCLB	36 12
105	RCL5	36 05	142	GTOa	22 16 11	179	RCLC	36 13
106	-	-45	143	9	09	180	+	-55
107	RCL6	36 06	144	RCLC	36 13	181	CHS	-22
108	+	-55	145	X>Y?	16-34	182	STOE	36 15
109	3	03	146	GTOa	22 16 11	183	DSP0	-63 00
110	÷	-24	147	X<0?	16-45	184	SPC	16-11
111	STOB	35 12	148	GTOa	22 16 11	185	RCLB	36 12
112	RCL4	36 04	149	FRC	16 44	186	PRTX	-14
113	RCL5	36 05	150	X#0?	16-42	187	RCLC	36 13
114	2	02	151	GTOa	22 16 11	188	PRTX	-14
115	x	-35	152	9	09	189	RCLC	36 15
116	+	-55	153	RCLD	36 14	190	PRTX	-14
117	RCL6	36 06	154	X>Y?	16-34	191	RCLD	36 14
118	+	-55	155	GTOa	22 16 11	192	PRTX	-14
119	3	03	156	X<0?	16-45	193	RTN	24
120	÷	-24	157	GTOa	22 16 11	194	*LBL2	21 02
121	STOC	35 13	158	FRC	16 44	195	RCL4	36 04
122	RCL4	36 04	159	X#0?	16-42	196	RCL6	36 06
123	2	02	160	GTOa	22 16 11	197	-	-45
124	x	-35	161	RCLB	36 12	198	STOB	35 12
125	CHS	-22	162	1	01	199	RCL5	36 05
126	RCL5	36 05	163	0	00	200	RCL4	36 04
127	-	-45	164	0	00	201	-	-45
128	RCL6	36 06	165	x	-35	202	STOC	35 13
129	+	-55	166	RCLC	36 13	203	RCL4	36 04
130	3	03	167	1	01	204	RCL5	36 05
131	÷	-24	168	0	00	205	+	-55
132	STOD	35 14	169	x	-35	206	RCL6	36 06
133	SPC	16-11	170	+	-55	207	+	-55
134	9	09	171	RCLD	36 14	208	STOD	35 14
135	RCLB	36 12	172	+	-55	209	RTN	24
136	X>Y?	16-34	173	DSP0	-63 00	210	R/S	51

Program 8: Monoclinic System Crystal Parameters

Program use- This program is used to calculate d spacings of crystal planes, interplanar angles, and interzonal angles for the monoclinic crystal system. The applicable formulas are:

$$\frac{1}{d^2} = \frac{h^2}{a^2 \sin^2 \beta} + \frac{k^2}{b^2} + \frac{l^2}{c^2 \sin^2 \beta} - \frac{2hl \cos \beta}{ac \sin^2 \beta}$$

$$\cos\phi = \frac{h_1 h_2 / a^2 + k_1 k_2 \sin^2 \beta / b^2 + l_1 l_2 / c^2 - (l_1 h_2 + l_2 h_1) \cos \beta / ac}{\left((h_1^2 / a^2 + k_1^2 \sin^2 \beta / b^2 + l_1^2 / c^2 - 2h_1 l_1 \cos \beta / ac)^{1/2} \times \right. \\ \left. (h_2^2 / a^2 + k_2^2 \sin^2 \beta / b^2 + l_2^2 / c^2 - 2h_2 l_2 \cos \beta / ac)^{1/2} \right)}$$

$$\cos\rho = \frac{a^2 u_1 u_2 + b^2 v_1 v_2 + c^2 w_1 w_2 + ac(w_1 u_2 + u_1 w_2) \cos \beta}{\left((a^2 u_1^2 + b^2 v_1^2 + c^2 w_1^2 + 2ac u_1 w_1 \cos \beta)^{1/2} \times \right. \\ \left. (a^2 u_2^2 + b^2 v_2^2 + c^2 w_2^2 + 2ac u_2 w_2 \cos \beta)^{1/2} \right)}$$

The input and output parameters are:

	Input parameters	Output parameters ^a	
Label A	Register 1- a	d	or d
Card 1	Register 2- b	hkl	h
Calculate d	Register 3- c		k
	Register 4- h		l
	Register 5- k		
	Register 6- l		
	Register B- β		
Label C	Register 1- a	d	or d
Card 1	Register 2- b	hkl	h
Calculate all possible d's within limits	Register 3- c		k
	Register 7- largest h to be printed		l
	Register 8- largest k to be printed		
	Register 9- largest l to be printed		
	Register B- β		
	Register E- only d values larger than this printed		
Label D	Register 1- a	ϕ	or ϕ
Card 2	Register 2- b	$h_1 k_1 l_1$	h_1
Calculate angle (ϕ) between crystal planes	Register 3- c	$h_2 k_2 l_2$	k_1
	Register 4- h_1		l_1
	Register 5- k_1		h_2
	Register 6- l_1		k_2
	Register 7- h_2		l_2
	Register 8- k_2		
	Register 9- l_2		
	Register B- β		

	Input parameters	Output parameters ^a
Label E	Register 1- a	ρ or ρ
Card 3	Register 2- b	$u_1 v_1 w_1$ or u_1
Calculate angle	Register 3- c	$u_2 v_2 w_2$ or v_1
(ρ) between	Register 4- u_1	w_1
crystal zones	Register 5- v_1	u_2
	Register 6- w_1	v_2
	Register 7- u_2	w_2
	Register 8- v_2	
	Register 9- w_2	
	Register B- β	

^aIf h, k, and l (u, v, and w) are 0 or positive and less than 10, output is in the form hkl (uvw). If h, k, or l (u, v, or w) are negative, or greater than 9, output

is in the form $\begin{matrix} h & u \\ k & \text{or } v \\ l & w \end{matrix}$.

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push D for Label D). The actual program follows.

Card 1. Monoclinic									
001	*LBLA	21	11	029	0	00	057	GSBD	23 14
002	GSB1	23	01	030	STO5	35 05	058	X=0?	16-43
003	PRTX	-14		031	STO6	35 06	059	GSBa	23 16 11
004	*LBLa	21	16 11	032	STOA	35 11	060	GTO0	22 00
005	DSP0	-63	00	033	STOC	35 13	061	*LBLB	21 12
006	9		09	034	STOD	35 14	062	1	01
007	RCL4	36	04	035	*LBL0	21 00	063	STOA	35 11
008	X>Y?	16-34		036	RCL9	36 09	064	*LBLc	21 16 13
009	GTOb	22	16 12	037	RCL6	36 06	065	RCLD	36 14
010	X<0?	16-45		038	X=Y?	16-33	066	X#0?	16-42
011	GTOb	22	16 12	039	GTOc	22 16 13	067	GTOc	22 16 13
012	GSB3	23	03	040	1	01	068	RCLC	36 13
013	GSB9	23	09	041	ST+6	35-55 06	069	X#0?	16-42
014	PRTX	-14		042	0	00	070	GTOE	22 15
015	RTN	24		043	STOC	35 13	071	*LBL6	21 06
016	*LBLb	21	16 12	044	STOD	35 14	072	RCL8	36 08
017	RCL4	36	04	045	*LBL7	21 07	073	RCL5	36 05
018	PRTX	-14		046	0	00	074	X=Y?	16-33
019	RCL5	36	05	047	STOA	35 11	075	GTOd	22 16 14
020	PRTX	-14		048	GSB1	23 01	076	RCLI	36 46
021	RCL6	36	06	049	RCLE	36 15	077	X#0?	16-42
022	PRTX	-14		050	X>Y?	16-34	078	GTO2	22 02
023	RTN	24		051	GTOB	22 12	079	1	01
024	*LBLE	21	13	052	X#Y	-41	080	STOC	35 13
025	0	00		053	SPC	16-11	081	ST+5	35-55 05
026	STO4	35	04	054	PRTX	-14	082	0	00
027	STOI	35	46	055	RCLI	36 46	083	STO6	35 06
028	*LBI.5	21	05	056	X#0?	16-42	084	GTO7	22 07

Card 1. Monoclinic (Concluded)

085	*LBLc	21	16	13	132	DSP4	-63	04	178	CHS	-22
086	RCLI	36	46		133	RCL4	36	04	179	PRTX	-14
087	X≠0?	16-42			134	RCLB	36	12	180	RTN	24
088	GTO4	22	04		135	SIN		41	181	*LBL3	21 03
089	RCLA	36	11		136	STO0	35	00	182	9	09
090	X=0?	16-43			137	÷		-24	183	RCL5	36 05
091	GTO6	22	06		138	RCL1	36	01	184	X>Y?	16-34
092	GTOe	22	16	15	139	÷		-24	185	GTOb	22 16 12
093	*LBLE	21	15		140	X ²		53	186	X<0?	16-45
094	RCLA	36	11		141	RCL5	36	05	187	GTOb	22 16 12
095	X=0?	16-43			142	RCL2	36	02	188	9	09
096	GTO6	22	06		143	÷		-24	189	RCL6	36 06
097	*LBLd	21	16	14	144	X ²		53	190	X>Y?	16-34
098	RCL7	36	07		145	+		-55	191	GTOb	22 16 12
099	RCL4	36	04		146	RCL6	36	06	192	X<0?	16-45
100	ABS	16	31		147	RCL0	36	00	193	GTOb	22 16 12
101	X=Y?	16-33			148	÷		-24	194	RCL4	36 04
102	GTOe	22	16	15	149	RCL3	36	03	195	1	01
103	0		00		150	÷		-24	196	0	00
104	STO5	35	05		151	X ²		53	197	0	00
105	1		01		152	+		-55	198	x	-35
106	STOD	35	14		153	RCL4	36	04	199	RTN	24
107	RCLI	36	46		154	2		02	200	*LBL9	21 09
108	X≠0?	16-42			155	x		-35	201	+	-55
109	GTO8	22	08		156	RCL6	36	06	202	RCL5	36 05
110	1		01		157	x		-35	203	1	01
111	ST+4	35-55	04		158	RCLB	36	12	204	0	00
112	0		00		159	COS		42	205	x	-35
113	STO6	35	06		160	x		-35	206	+	-55
114	GTO7	22	07		161	RCL1	36	01	207	RTN	24
115	*LBLe	21	16	15	162	÷		-24	208	*LBL2	21 02
116	RCLI	36	46		163	RCL3	36	03	209	1	01
117	X≠0?	16-42			164	÷		-24	210	STO6	35 06
118	R/S		51		165	RCL0	36	00	211	STOC	35 13
119	1		01		166	X ²		53	212	ST+5	35-55 05
120	STOI	35	46		167	÷		-24	213	GTO7	22 07
121	RCL7	36	07		168	-		-45	214	*LBL4	21 04
122	X=0?	16-43			169	1/X		52	215	RCLA	36 11
123	R/S		51		170	ABS	16	31	216	X≠0?	16-42
124	RCL9	36	09		171	√X		54	217	R/S	51
125	X=0?	16-43			172	RTN		24	218	GTO6	22 06
126	R/S		51		173	*LBLD	21	14	219	*LBL8	21 08
127	1		01		174	DSP0	-63	00	220	1	01
128	CHS	-22			175	GSB3	23	03	221	STO6	35 06
129	STO4	35	04		176	CHS		-22	222	ST-4	35-45 04
130	GTO5	22	05		177	GSB9	23	09	223	GTO7	22 07
131	*LBL1	21	01								

Card 2. Monoclinic

001	*LBLD	21 14	052	+	-55	103	GTOb	22 16 12
002	RCL4	36 04	053	RCL4	36 04	104	X<0?	16-45
003	RCL7	36 07	054	RCL6	36 06	105	GTOb	22 16 12
004	x	-35	055	GSB6	23 06	106	RCL4	36 04
005	RCL1	36 01	056	STOA	35 11	107	1	01
006	X ²	53	057	RCL7	36 07	108	0	00
007	÷	-24	058	RCL1	36 01	109	0	00
008	RCL5	36 05	059	÷	-24	110	x	-35
009	RCL8	36 08	060	X ²	53	111	+	-55
010	x	-35	061	RCL8	36 08	112	RCL5	36 05
011	RCL2	36 02	062	GSB5	23 05	113	1	01
012	X ²	53	063	RCL9	36 09	114	0	00
013	÷	-24	064	RCL3	36 03	115	x	-35
014	RCLB	36 12	065	÷	-24	116	+	-55
015	SIN	41	066	X ²	53	117	PRTX	-14
016	X ²	53	067	+	-55	118	GTOc	22 16 13
017	x	-35	068	RCL7	36 07	119	*LBLb	21 16 12
018	+	-55	069	RCL9	36 09	120	RCL4	36 04
019	RCL6	36 06	070	GSB6	23 06	121	PRTX	-14
020	RCL9	36 09	071	RCLA	36 11	122	RCL5	36 05
021	x	-35	072	x	-35	123	PRTX	-14
022	RCL3	36 03	073	ABS	16 31	124	RCL6	36 06
023	X ²	53	074	√X	54	125	PRTX	-14
024	÷	-24	075	RCL0	36 00	126	*LBLc	21 16 13
025	+	-55	076	X≠Y	-41	127	9	09
026	RCL6	36 06	077	÷	-24	128	RCL7	36 07
027	RCL7	36 07	078	COS ⁻¹	16 42	129	X>Y?	16-34
028	x	-35	079	9	09	130	GTOd	22 16 14
029	RCL9	36 09	080	0	00	131	X<0?	16-45
030	RCL4	36 04	081	X≠Y	-41	132	GTOd	22 16 14
031	x	-35	082	X>Y?	16-34	133	9	09
032	+	-55	083	GSB1	23 01	134	RCL8	36 08
033	RCLB	36 12	084	SPC	16-11	135	X>Y?	16-34
034	COS	42	085	DSP2	-63 02	136	GTOd	22 16 14
035	x	-35	086	PRTX	-14	137	X<0?	16-45
036	RCL1	36 01	087	DSP0	-63 00	138	GTOd	22 16 14
037	RCL3	36 03	088	9	09	139	9	09
038	x	-35	089	RCL4	36 04	140	RCL9	36 09
039	÷	-24	090	X>Y?	16-34	141	X>Y?	16-34
040	-	-45	091	GTOb	22 16 12	142	GTOd	22 16 14
041	STO0	35 00	092	X<0?	16-45	143	X<0?	16-45
042	RCL4	36 04	093	GTOb	22 16 12	144	GTOd	22 16 14
043	RCL1	36 01	094	9	09	145	RCL7	36 07
044	÷	-24	095	RCL5	36 05	146	1	01
045	X ²	53	096	X>Y?	16-34	147	0	00
046	RCL5	36 05	097	GTOb	22 16 12	148	0	00
047	GSB5	23 05	098	X<0?	16-45	149	x	-35
048	RCL6	36 06	099	GTOb	22 16 12	150	+	-55
049	RCL3	36 03	100	9	09	151	RCL8	36 08
050	÷	-24	101	RCL6	36 06	152	1	01
051	X ²	53	102	X>Y?	16-34	153	0	00

Card 2. Monoclinic (Concluded)

154	x	-35	168	÷	-24	182	÷	-24
155	+	-55	169	RCLB	36 12	183	RCLB	36 12
156	PRTX	-14	170	SIN	41	184	COS	42
157	RTN	24	171	x	-35	185	x	-35
158	*LBLd	21 16 14	172	X ²	53	186	-	-45
159	RCL7	36 07	173	+	-55	187	RTN	24
160	PRTX	-14	174	RTN	24	188	*LBL1	21 01
161	RCL8	36 08	175	*LBL6	21 06	189	1	01
162	PRTX	-14	176	x	-35	190	8	08
163	RCL9	36 09	177	2	02	191	0	00
164	PRTX	-14	178	x	-35	192	X=Y	-41
165	RTN	24	179	RCL1	36 01	193	-	-45
166	*LBL5	21 05	180	÷	-24	194	RTN	24
167	RCL2	36 02	181	RCL3	36 03	195	R/S	51

Card 3. Monoclinic

001	*LBL5	21 15	036	+	-55	071	x	-35
002	RCL4	36 04	037	STO0	35 00	072	+	-55
003	RCL7	36 07	038	RCL4	36 04	073	RCLA	36 11
004	x	-35	039	RCL1	36 01	074	x	-35
005	RCL1	36 01	040	x	-35	075	ABS	16 31
006	X ²	53	041	X ²	53	076	√X	54
007	x	-35	042	RCL5	36 05	077	RCL0	36 00
008	RCL5	36 05	043	RCL2	36 02	078	X=Y	-41
009	RCL8	36 08	044	x	-35	079	÷	-24
010	x	-35	045	X ²	53	080	COS ⁻¹	16 42
011	RCL2	36 02	046	+	-55	081	9	09
012	X ²	53	047	RCL6	36 06	082	0	00
013	x	-35	048	RCL3	36 03	083	X=Y	-41
014	+	-55	049	GSB7	23 07	084	X>Y?	16-34
015	RCL6	36 06	050	RCL4	36 04	085	GSB1	23 01
016	RCL9	36 09	051	x	-35	086	SPC	16-11
017	x	-35	052	RCL6	36 06	087	DSP2	-63 02
018	RCL3	36 03	053	x	-35	088	PRTX	-14
019	X ²	53	054	+	-55	089	DSP0	-63 00
020	x	-35	055	STOA	35 11	090	9	09
021	+	-55	056	RCL7	36 07	091	RCL4	36 04
022	RCL6	36 06	057	RCL1	36 01	092	X>Y?	16-34
023	RCL7	36 07	058	x	-35	093	GTOb	22 16 12
024	x	-35	059	X ²	53	094	X<0?	16-45
025	RCL9	36 09	060	RCL8	36 08	095	GTOb	22 16 12
026	RCL4	36 04	061	RCL2	36 02	096	9	09
027	x	-35	062	x	-35	097	RCL5	36 05
028	+	-55	063	X ²	53	098	X>Y?	16-34
029	RCLB	36 12	064	+	-55	099	GTOb	22 16 12
030	COS	42	065	RCL9	36 09	100	X<0?	16-45
031	x	-35	066	RCL3	36 03	101	GTOb	22 16 12
032	RCL1	36 01	067	GSB7	23 07	102	9	09
033	RCL3	36 03	068	RCL7	36 07	103	RCL6	36 06
034	x	-35	069	x	-35	104	X>Y?	16-34
035	x	-35	070	RCL9	36 09	105	GTOb	22 16 12

Card 3. Monoclinic (Concluded)

106	X<0?	16-45	134	GTOd	22 16 14	162	PRTX	-14
107	GTOb	22 16 12	135	9	09	163	RCL8	36 08
108	RCL4	36 04	136	RCL8	36 08	164	PRTX	-14
109	1	01	137	X>Y?	16-34	165	RCL9	36 09
110	0	00	138	GTOd	22 16 14	166	PRTX	-14
111	0	00	139	X<0?	16-45	167	RTN	24
112	x	-35	140	GTOd	22 16 14	168	*LBL7	21 07
113	+	-55	141	9	09	169	x	-35
114	RCL5	36 05	142	RCL9	36 09	170	X ²	53
115	1	01	143	X>Y?	16-34	171	+	-55
116	0	00	144	GTOd	22 16 14	172	RCL1	36 01
117	x	-35	145	X<0?	16-45	173	2	02
118	+	-55	146	GTOd	22 16 14	174	x	-35
119	PRTX	-14	147	RCL7	36 07	175	RCL3	36 03
120	GTOc	22 16 13	148	1	01	176	x	-35
121	*LBLb	21 16 12	149	0	00	177	RCLB	36 12
122	RCL4	36 04	150	0	00	178	COS	42
123	PRTX	-14	151	x	-35	179	x	-35
124	RCL5	36 05	152	+	-55	180	RTN	24
125	PRTX	-14	153	RCL8	36 08	181	*LBL1	21 01
126	RCL6	36 06	154	1	01	182	1	01
127	PRTX	-14	155	0	00	183	8	08
128	*LBLc	21 16 13	156	x	-35	184	0	00
129	9	09	157	+	-55	185	X≠Y	-41
130	RCL7	36 07	158	PRTX	-14	186	-	-45
131	X>Y?	16-34	159	RTN	24	187	RTN	24
132	GTOd	22 16 14	160	*LBLd	21 16 14	188	R/S	51
133	X<0?	16-45	161	RCL7	36 07			

Program 9: Triclinic System Crystal Parameters

Program use- This program is used to calculate d spacings of crystal planes, interplanar angles, and interzonal angles for the triclinic crystal system. The applicable formulas are:

$$\frac{1}{d^2} = \frac{1}{V^2} (s_{11}h^2 + s_{22}k^2 + s_{33}l^2 + 2s_{12}hk + 2s_{23}kl + 2s_{31}lh)$$

where

$$V^2 = a^2b^2c^2(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)$$

$$s_{11} = b^2c^2\sin^2\alpha$$

$$s_{22} = a^2c^2\sin^2\beta$$

$$s_{33} = a^2b^2\sin^2\gamma$$

$$s_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$$

$$s_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$$

$$s_{31} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$$

$$\cos\phi = \frac{F}{A_{h_1k_1l_1} \cdot A_{h_2k_2l_2}}$$

where

$$F = h_1h_2b^2c^2\sin^2\alpha + k_1k_2a^2c^2\sin^2\beta + l_1l_2a^2b^2\sin^2\gamma$$

$$+ abc^2(\cos\alpha\cos\beta - \cos\gamma)(k_1h_2 + h_1k_2)$$

$$+ ab^2c(\cos\gamma\cos\alpha - \cos\beta)(h_1l_2 + l_1h_2)$$

$$+ a^2bc(\cos\beta\cos\gamma - \cos\alpha)(k_1l_2 + l_1k_2)$$

and

$$A_{hkl} = [h^2b^2c^2\sin^2\alpha + k^2a^2c^2\sin^2\beta + l^2a^2b^2\sin^2\gamma$$

$$+ 2hkabc^2(\cos\alpha\cos\beta - \cos\gamma)$$

$$+ 2hlab^2c(\cos\gamma\cos\alpha - \cos\beta)$$

$$+ 2kla^2bc(\cos\beta\cos\gamma - \cos\alpha)]^{1/2}$$

$$\cos\psi = \frac{L}{I_{u_1v_1w_1} \cdot I_{u_2v_2w_2}}$$

where

$$L = a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2$$

$$+ bc(v_1w_2 + w_1v_2)\cos\alpha$$

$$+ ac(w_1u_2 + u_1w_2)\cos\beta$$

$$+ ab(u_1v_2 + v_1u_2)\cos\gamma$$

and

$$I_{uvw} = (a^2u^2 + b^2v^2 + c^2w^2 + 2bcvw\cos\alpha + 2cawu\cos\beta + 2abuv\cos\gamma)^{1/2}$$

The input and output parameters are:

	Input parameters	Output parameters		
Label A	Register 1- a	d		
Card 1	Register 2- b	h		
Calculate d	Register 3- c	k		
	Register 4- h	l		
	Register 5- k			
	Register 6- l			
	Register A- α			
	Register B- β			
	Register C- γ			
Label C	Register 1- a	d		
Card 1	Register 2- b	h		
Calculate all possible d's within limits	Register 3- c	k		
	Register 7- largest h to be printed	l		
	Register 8- largest k to be printed			
	Register 9- largest l to be printed			
	Register A- α			
	Register B- β			
	Register C- γ			
	Register E- only d values larger than this printed			
	Label D ^{α}	Register 1- a	ϕ	or ϕ
	Card 2	Register 2- b	$h_1 k_1 l_1$	h_1
Calculate angle (ϕ) between crystal planes	Register 3- c	h_2	k_1	
	Register 4- h_1	k_2	l_1	
	Register 5- k_1	l_2	h_2	
	Register 6- l_1		k_2	
	Register 7- h_2		l_2	
	Register 8- k_2			
	Register 9- l_2			
	Register A- α			
	Register B- β			
	Register C- γ			
Label E ^{α}	Register 1- a	ρ	or ρ	
Card 3	Register 2- b	$u_1 v_1 w_1$	u_1	
Calculate angle (ρ) between crystal zones	Register 3- c	$u_2 v_2 w_2$	v_1	
	Register 4- u_1		w_1	
	Register 5- v_1		u_2	
	Register 6- w_1		v_2	
	Register 7- u_2		w_2	
	Register 8- v_2			
	Register 9- w_2			
	Register A- α			

Input parameters Output parameters
 Register B- β
 Register C- γ

^aIf h, k, and l (u, v, and w) are zero or positive and less than 10, output is in the form hkl (uvw). If h, k, or l (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h & u \\ k & \text{or } v \\ l & w \end{matrix}$.

This program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push A for Label A). The actual program follows.

Card 1. Triclinic													
001	*LBLA	21	11	036	RCL5	36	05	071	CHS	-22			
002	GSBe	23	16	15	+		-55	072	STO5	35	05		
003	*LBLc	21	16	13	038	X=0?	16-43	073	RCL6	36	06		
004	SPC		16-11	039	GTO5	22	05	074	X=0?	16-43			
005	DSP4	-63	04	040	RCL6	36	06	075	GTO5	22	05		
006	PRTX		-14	041	CHS		-22	076	RCL4	36	04		
007	DSP0	-63	00	042	STO6	35	06	077	CHS		-22		
008	RCL4	36	04	043	X=0?		16-43	078	STO4	35	04		
009	PRTX		-14	044	GTOd	22	16	14	079	GSBe	23	16	15
010	RCL5	36	05	045	GSBe	23	16	15	080	RCL6	36	15	
011	PRTX		-14	046	RCL6	36	15		081	X>Y?	16-34		
012	RCL6	36	06	047	X>Y?		16-34		082	GTOE	22	15	
013	PRTX		-14	048	GTOd	22	16	14	083	X=Y		-41	
014	RTN		24	049	X=Y		-41		084	GSBe	23	16	13
015	*LBLC	21	13	050	GSBe	23	16	13	085	*LBL6	21	15	
016	0		00	051	*LBLd	21	16	14	086	RCL4	36	04	
017	STO4	35	04	052	RCL6	36	06		087	CHS		-22	
018	STO5	35	05	053	CHS		-22		088	STO4	35	04	
019	STO6	35	06	054	STO6	35	06		089	GTO5	22	05	
020	*LBL5	21	05	055	RCL4	36	04		090	*LBL9	21	09	
021	RCL9	36	09	056	X=0?		16-43		091	RCL8	36	08	
022	RCL6	36	06	057	GTO5	22	05		092	RCL5	36	05	
023	X=Y?	16-33		058	RCL5	36	05		093	X=Y?	16-33		
024	GTO9	22	09	059	X=0?		16-43		094	GTO8	22	08	
025	1		01	060	GTO5	22	05		095	1		01	
026	ST+6	35-55	06	061	CHS		-22		096	ST+5	35-55	05	
027	*LBL6	21	06	062	STO5	35	05		097	0		00	
028	GSBe	23	16	15	063	GSBe	23	16	13	098	STO6	35	06
029	RCL6	36	15	064	RCL6	36	15		099	GTO6	22	06	
030	X>Y?	16-34		065	X>Y?		16-34		100	*LBL8	21	08	
031	GTO4	22	04	066	GTO3	22	03		101	RCL7	36	07	
032	X=Y		-41	067	X=Y		-41		102	RCL4	36	04	
033	GSBe	23	16	13	068	GSBe	23	16	13	103	X=Y?	16-33	
034	*LBL4	21	04	069	*LBL3	21	03		104	R/S		51	
035	RCL4	36	04	070	RCL5	36	05		105	1		01	

Card 1. Triclinic (Concluded)

106	ST+4	35-55	04	143	RCL1	36 01	180	RCL6	36 06
107	0		00	144	RCL2	36 02	181	GSB2	23 02
108	STO5	35	05	145	x	-35	182	RCLI	36 46
109	STO6	35	06	146	RCLC	36 13	183	RCL0	36 00
110	GTO6	22	06	147	SIN	41	184	x	-35
111	*LBL1	21	01	148	x	-35	185	RCLD	36 14
112	RCL1	36	01	149	RCL6	36 06	186	-	-45
113	x		-35	150	x	-35	187	GSB1	23 01
114	*LBLb	21	16 12	151	X ²	53	188	RCL2	36 02
115	RCL2	36	02	152	+	-55	189	x	-35
116	x		-35	153	RCLA	36 11	190	RCL6	36 06
117	*LBLa	21	16 11	154	COS	42	191	x	-35
118	RCL3	36	03	155	STO0	35 00	192	RCL4	36 04
119	x		-35	156	RCLB	36 12	193	GSB2	23 02
120	RTN		24	157	COS	42	194	RCL0	36 00
121	*LBL2	21	02	158	STOD	35 14	195	X ²	53
122	x		-35	159	x	-35	196	CHS	-22
123	2		02	160	RCLC	36 13	197	1	01
124	x		-35	161	COS	42	198	+	-55
125	+		-55	162	STOI	35 46	199	RCLD	36 14
126	RTN		24	163	-	-45	200	X ²	53
127	*LBLe	21	16 15	164	GSB1	23 01	201	-	-45
128	RCLA	36	11	165	GSBa	23 16 11	202	RCLI	36 46
129	SIN		41	166	RCL4	36 04	203	X ²	53
130	GSBb	23	16 12	167	x	-35	204	-	-45
131	RCL4	36	04	168	RCL5	36 05	205	RCL0	36 00
132	x		-35	169	GSB2	23 02	206	RCLD	36 14
133	X ²		53	170	RCLD	36 14	207	x	-35
134	RCL1	36	01	171	RCLI	36 46	208	RCLI	36 46
135	GSBa	23	16 11	172	x	-35	209	GSB2	23 02
136	RCLB	36	12	173	RCL0	36 00	210	GSB1	23 01
137	SIN		41	174	-	-45	211	GSB1	23 01
138	x		-35	175	GSB1	23 01	212	X ² =Y	-41
139	RCL5	36	05	176	RCL1	36 01	213	÷	-24
140	x		-35	177	x	-35	214	ABS	16 31
141	X ²		53	178	RCL5	36 05	215	√X	54
142	+		-55	179	x	-35	216	RTN	24

Card 2. Triclinic

001	*LBLD	21	14	013	GSBe	23 16 15	025	RCL8	36 08
002	RCL4	36	04	014	RCL5	36 05	026	GSBd	23 16 14
003	GSBa	23	16 11	015	RCL6	36 06	027	RCL7	36 07
004	RCL5	36	05	016	GSBE	23 15	028	RCL9	36 09
005	GSBb	23	16 12	017	STOI	35 46	029	GSBe	23 16 15
006	RCL6	36	06	018	RCL7	36 07	030	RCL8	36 08
007	GSBc	23	16 13	019	GSBa	23 16 11	031	RCL9	36 09
008	RCL4	36	04	020	RCL8	36 08	032	GSBE	23 15
009	RCL5	36	05	021	GSBb	23 16 12	033	RCLI	36 46
010	GSBd	23	16 14	022	RCL9	36 09	034	x	-35
011	RCL4	36	04	023	GSBc	23 16 13	035	ABS	16 31
012	RCL6	36	06	024	RCL7	36 07	036	√X	54

Card 2. Triclinic (Continued)

037	STOI	35 46	088	GSB4	23 04	139	GSBA	23 11
038	RCL2	36 02	089	RCLI	36 46	140	RTN	24
039	GSBA	23 11	090	÷	-24	141	*LBLa	21 16 11
040	RCLA	36 11	091	COS ⁻¹	16 42	142	GSBB	23 12
041	SIN	41	092	PRTX	-14	143	GSBA	23 11
042	GSB6	23 06	093	RCL4	36 04	144	RCLA	36 11
043	RCL4	36 04	094	X<0?	16-45	145	SIN	41
044	x	-35	095	GTO8	22 08	146	GSB6	23 06
045	RCL7	36 07	096	9	09	147	RTN	24
046	x	-35	097	RCL5	36 05	148	*LBLb	21 16 12
047	RCL1	36 01	098	X>Y?	16-34	149	RCL1	36 01
048	GSBA	23 11	099	GTO8	22 08	150	x	-35
049	RCLB	36 12	100	X<0?	16-45	151	GSBA	23 11
050	SIN	41	101	GTO8	22 08	152	RCLB	36 12
051	GSB6	23 06	102	9	09	153	SIN	41
052	RCL5	36 05	103	RCL6	36 06	154	GSB6	23 06
053	x	-35	104	X>Y?	16-34	155	+	-55
054	RCL8	36 08	105	GTO8	22 08	156	RTN	24
055	GSB7	23 07	106	X<0?	16-45	157	*LBLc	21 16 13
056	RCL1	36 01	107	GTO8	22 08	158	RCL1	36 01
057	GSBB	23 12	108	RCL4	36 04	159	x	-35
058	RCLC	36 13	109	1	01	160	GSBB	23 12
059	SIN	41	110	0	00	161	RCLC	36 13
060	GSB6	23 06	111	0	00'	162	SIN	41
061	RCL6	36 06	112	GSB7	23 07	163	GSB6	23 06
062	x	-35	113	RCL5	36 05	164	+	-55
063	RCL9	36 09	114	1	01	165	RTN	24
064	GSB7	23 07	115	0	00	166	*LBLd	21 16 14
065	RCL5	36 05	116	GSB7	23 07	167	x	-35
066	RCL7	36 07	117	PRTX	-14	168	GSBA	23 11
067	x	-35	118	*LBL9	21 09	169	2	02
068	RCL4	36 04	119	RCL7	36 07	170	*LBL2	21 02
069	RCL8	36 08	120	PRTX	-14	171	GSB1	23 01
070	GSB7	23 07	121	RCL8	36 08	172	RCLA	36 11
071	RCL3	36 03	122	PRTX	-14	173	COS	42
072	GSB2	23 02	123	RCL9	36 09	174	STOD	35 14
073	RCL4	36 04	124	PRTX	-14	175	RCLB	36 12
074	RCL9	36 09	125	RTN	24	176	COS	42
075	x	-35	126	*LBL8	21 08	177	STOE	35 15
076	RCL6	36 06	127	RCL4	36 04	178	x	-35
077	RCL7	36 07	128	PRTX	-14	179	RCLC	36 13
078	GSB7	23 07	129	RCL5	36 05	180	COS	42
079	RCL2	36 02	130	PRTX	-14	181	STO0	35 00
080	GSB3	23 03	131	RCL6	36 06	182	GTO5	22 05
081	RCL5	36 05	132	PRTX	-14	183	*LBLe	21 16 15
082	RCL9	36 09	133	GTO9	22 09	184	x	-35
083	x	-35	134	*LBL1	21 01	185	GSBB	23 12
084	RCL6	36 06	135	x	-35	186	2	02
085	RCL8	36 08	136	RCL1	36 01	187	*LBL3	21 03
086	GSB7	23 07	137	x	-35	188	GSB1	23 01
087	RCL1	36 01	138	GSBB	23 12	189	RCL0	36 00

Card 2. Triclinic (Concluded)

190	RCLD	36 14	202	RCL0	36 00	214	x	-35
191	x	-35	203	x	-35	215	+	-55
192	RCLD	36 15	204	RCLD	36 14	216	RTN	24
193	GTO5	22 05	205	*LBL5	21 05	217	*LBLA	21 11
194	*LBLD	21 15	206	-	-45	218	RCL3	36 03
195	x	-35	207	GSB7	23 07	219	x	-35
196	RCL1	36 01	208	RTN	24	220	RTN	24
197	x	-35	209	*LBL6	21 06	221	*LBLB	21 12
198	2	02	210	x	-35	222	RCL2	36 02
199	*LBL4	21 04	211	X ²	53	223	x	-35
200	GSB1	23 01	212	RTN	24	224	RTN	24
201	RCLD	36 15	213	*LBL7	21 07			

Card 3. Triclinic

001	*LBLD	21 15	038	RCL7	36 07	075	RCL9	36 09
002	RCL4	36 04	039	GSBb	23 16 12	076	RCL3	36 03
003	RCL7	36 07	040	GSB3	23 03	077	GSBa	23 16 11
004	x	-35	041	STO0	35 00	078	RCL8	36 08
005	RCL1	36 01	042	RCL4	36 04	079	GSBc	23 16 13
006	X ²	53	043	RCL1	36 01	080	RCL9	36 09
007	x	-35	044	x	-35	081	x	-35
008	RCL5	36 05	045	X ²	53	082	GSB1	23 01
009	RCL8	36 08	046	RCL5	36 05	083	RCL7	36 07
010	x	-35	047	RCL2	36 02	084	GSBc	23 16 13
011	RCL2	36 02	048	GSBa	23 16 11	085	RCL9	36 09
012	X ²	53	049	RCL6	36 06	086	x	-35
013	GSBb	23 16 12	050	RCL3	36 03	087	GSB2	23 02
014	RCL6	36 06	051	GSBa	23 16 11	088	RCL7	36 07
015	RCL9	36 09	052	RCL5	36 05	089	GSBc	23 16 13
016	x	-35	053	GSBc	23 16 13	090	RCL8	36 08
017	RCL3	36 03	054	RCL6	36 06	091	x	-35
018	X ²	53	055	x	-35	092	GSB3	23 03
019	GSBb	23 16 12	056	GSB1	23 01	093	RCL1	36 46
020	RCL5	36 05	057	RCL4	36 04	094	x	-35
021	RCL9	36 09	058	GSBc	23 16 13	095	ABS	16 31
022	x	-35	059	RCL6	36 06	096	√X	54
023	RCL6	36 06	060	x	-35	097	RCL0	36 00
024	RCL8	36 08	061	GSB2	23 02	098	X≠Y	-41
025	GSBb	23 16 12	062	RCL4	36 04	099	÷	-24
026	GSB1	23 01	063	GSBc	23 16 13	100	COS ⁻¹	16 42
027	RCL6	36 06	064	RCL5	36 05	101	SPC	16-11
028	RCL7	36 07	065	x	-35	102	DSP2	-63 02
029	x	-35	066	GSB3	23 03	103	PRTX	-14
030	RCL4	36 04	067	STOI	35 46	104	DSP0	-63 00
031	RCL9	36 09	068	RCL7	36 07	105	9	09
032	GSBb	23 16 12	069	RCL1	36 01	106	RCL4	36 04
033	GSB2	23 02	070	x	-35	107	X>Y?	16-34
034	RCL4	36 04	071	X ²	53	108	GTO7	22 07
035	RCL8	36 08	072	RCL8	36 08	109	X<0?	16-45
036	x	-35	073	RCL2	36 02	110	GTO7	22 07
037	RCL5	36 05	074	GSBa	23 16 11	111	9	09

Card 3. Triclinic (Concluded)

112	RCL5	36 05	150	9	09	187	RCL2	36 02
113	X>Y?	16-34	151	RCL8	36 08	188	x	-35
114	GTO7	22 07	152	X>Y?	16-34	189	RCL3	36 03
115	X<0?	16-45	153	GTO9	22 09	190	GSBb	23 16 12
116	GTO7	22 07	154	X<0?	16-45	191	RTN	24
117	9	09	155	GTO9	22 09	192	*LBL2	21 02
118	RCL6	36 06	156	9	09	193	RCLB	36 12
119	X>Y?	16-34	157	RCL9	36 09	194	COS	42
120	GTO7	22 07	158	X>Y?	16-34	195	x	-35
121	X<0?	16-45	159	GTO9	22 09	196	RCL1	36 01
122	GTO7	22 07	160	X<0?	16-45	197	x	-35
123	RCL4	36 04	161	GTO9	22 09	198	RCL3	36 03
124	1	01	162	RCL7	36 07	199	GSBb	23 16 12
125	0	00	163	1	01	200	RTN	24
126	0	00	164	0	00	201	*LBL3	21 03
127	x	-35	165	0	00	202	RCLC	36 13
128	+	-55	166	x	-35	203	COS	42
129	RCL5	36 05	167	+	-55	204	x	-35
130	1	01	168	RCL8	36 08	205	RCL1	36 01
131	0	00	169	1	01	206	x	-35
132	x	-35	170	0	00	207	RCL2	36 02
133	+	-55	171	x	-35	208	GSBb	23 16 12
134	PRTX	-14	172	+	-55	209	RTN	24
135	GTO8	22 08	173	PRTX	-14	210	*LBLa	21 16 11
136	*LBL7	21 07	174	RTN	24	211	x	-35
137	RCL4	36 04	175	*LBL9	21 09	212	X ²	53
138	PRTX	-14	176	RCL7	36 07	213	+	-55
139	RCL5	36 05	177	PRTX	-14	214	RTN	24
140	PRTX	-14	178	RCL8	36 08	215	*LBLb	21 16 12
141	RCL6	36 06	179	PRTX	-14	216	x	-35
142	PRTX	-14	180	RCL9	36 09	217	+	-55
143	*LBL8	21 08	181	PRTX	-14	218	RTN	24
144	9	09	182	RTN	24	219	*LBLc	21 16 13
145	RCL7	36 07	183	*LBL1	21 01	220	2	02
146	X>Y?	16-34	184	RCLA	36 11	221	x	-35
147	GTO9	22 09	185	COS	42	222	RTN	24
148	X<0?	16-45	186	x	-35	223	R/S	51
149	GTO9	22 09						

Program 10: Dealing with Apparent Crystal Parameters (Axial Angles and Lengths) Found on Electron Diffraction Patterns

Program use- This program is used to calculate apparent crystallographic parameters, as may be found on electron diffraction patterns of nonorthogonal crystals, from the known parameters of standard phases. The applicable formulas are:

Hexagonal: $a' = a(3/4)^{1/2}$

Rhombohedral:
$$a' = a \left(1 - \frac{2\cos\alpha_{rh}}{1 + \cos\alpha_{rh}} \right)^{1/2}$$

$$\cos\alpha' = \frac{(3a_{hex}^2/4c_{hex}^2) - 1/2}{(3a_{hex}^2/4c_{hex}^2) + 1}$$

Monoclinic: $a' = a\sin\beta$

$$c' = c\sin\beta$$

Triclinic: $a' = \frac{a}{\sin\alpha} (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$

$$b' = \frac{b}{\sin\beta} (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

$$c' = \frac{c}{\sin\gamma} (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

$$\cos\alpha' = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$$

$$\cos\beta' = \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma}$$

$$\cos\gamma' = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

The input and output parameters are:

	Input parameters	Output parameters
Label A	Register 1- α	a
TRICLINIC	Register 2- β	b
	Register 3- γ	c
	Register 4- a	α
	Register 5- b	β
	Register 6- c	γ
		$b'(\partial_{010})$
		$c'(\partial_{001})$
		α'
		β'
		γ'
Label B	Register 2- β	a
MONOCLINIC	Register 4- a	b
	Register 5- b	c
	Register 6- c	β

	Input parameters	Output parameters
		$a'(\partial_{100})$
		$b(\partial_{010})$
		$c'(\partial_{001})$
		β
Label C	Register 1- α_{rh}	a_{hex}
RHOMBOHEDRAL	Register 4- a_{hex}	c_{hex}
	Register 5- a_{rh}	a_{rh}
	Register 6- c_{hex}	α_{rh}
		$a'_{rh}(\partial_{001})$
		α'_{rh}
Label D	Register 4- a	a
HEXAGONAL	Register 6- c	c
		$a'(\partial_{100})$
		$c(\partial_{001})$

The program can be executed as many times as desired by storing the indicated input crystal parameters in their respective registers, and then pushing the appropriate label button (e.g., push A for Label A). The actual program follows.

Apparent Crystal Parameters												
001	*LBLA	21	11	026	RCL1	36	01	051	SIN	41		
002	GSB1	23	01	027	COS		42	052	÷	-24		
003	RCL1	36	01	028	RCL3	36	03	053	RCL2	36	02	
004	GSB5	23	05	029	COS		42	054	SIN		41	
005	RCL2	36	02	030	x		-35	055	÷		-24	
006	PRTX		-14	031	RCL2	36	02	056	COS^{-1}		16	42
007	RCL3	36	03	032	COS		42	057	STO9		35	09
008	PRTX		-14	033	-		-45	058	1			01
009	GSB7	23	07	034	RCL1	36	01	059	ENT↑			-21
010	RCL2	36	02	035	SIN		41	060	RCL1		36	01
011	COS		42	036	÷		-24	061	COS			42
012	RCL3	36	03	037	RCL3	36	03	062	X^2			53
013	COS		42	038	SIN		41	063	-			-45
014	x		-35	039	÷		-24	064	RCL2		36	02
015	RCL1	36	01	040	COS^{-1}		16	42	065	COS		42
016	COS		42	041	STO8		35	08	066	X^2		53
017	-		-45	042	RCL1	36	01	067	-			-45
018	RCL2	36	02	043	COS		42	068	RCL3		36	03
019	SIN		41	044	RCL2	36	02	069	COS			42
020	÷		-24	045	COS		42	070	X^2			53
021	RCL3	36	03	046	x		-35	071	-			-45
022	SIN		41	047	RCL3	36	03	072	RCL1		36	01
023	÷		-24	048	COS		42	073	COS			42
024	COS^{-1}		16	42	049	-	-45	074	2			02
025	STO7		35	07	050	RCL1	36	01	075	x		-35

Apparent Crystal Parameters (Continued)

076	RCL2	36 02	123	*LBLC	21 13	170	PRTX	-14
077	COS	42	124	GSB6	23 06	171	SPC	16-11
078	x	-35	125	RCL4	36 04	172	3	03
079	RCL3	36 03	126	GSB4	23 04	173	ENT↑	-21
080	COS	42	127	RCL6	36 06	174	4	04
081	x	-35	128	PRTX	-14	175	÷	-24
082	+	-55	129	SPC	16-11	176	√X	54
083	√X	54	130	RCL5	36 05	177	RCL4	36 04
084	STO0	35 00	131	PRTX	-14	178	x	-35
085	RCL4	36 04	132	RCL1	36 01	179	PRTX	-14
086	RCL1	36 01	133	GSB5	23 05	180	RCL6	36 06
087	GSB2	23 02	134	GSB7	23 07	181	PRTX	-14
088	RCL5	36 05	135	GSB3	23 03	182	RTN	24
089	RCL2	36 02	136	.	-62	183	*LBL1	21 01
090	GSB2	23 02	137	5	05	184	GSB6	23 06
091	RCL6	36 06	138	-	-45	185	RCL4	36 04
092	RCL3	36 03	139	GSB3	23 03	186	GSB4	23 04
093	GSB2	23 02	140	1	01	187	RCL5	36 05
094	SPC	16-11	141	+	-55	188	PRTX	-14
095	RCL7	36 07	142	÷	-24	189	RCL6	36 06
096	GSB5	23 05	143	COS ⁻¹	16 42	190	PRTX	-14
097	RCL8	36 08	144	STOI	35 46	191	SPC	16-11
098	PRTX	-14	145	RCL1	36 01	192	RTN	24
099	RCL9	36 09	146	COS	42	193	*LBL2	21 02
100	PRTX	-14	147	X ²	53	194	SIN	41
101	RTN	24	148	2	02	195	÷	-24
102	*LBLB	21 12	149	x	-35	196	RCL0	36 00
103	GSB1	23 01	150	RCL1	36 01	197	x	-35
104	RCL2	36 02	151	COS	42	198	GSB4	23 04
105	GSB5	23 05	152	1	01	199	RTN	24
106	GSB7	23 07	153	+	-55	200	*LBL3	21 03
107	RCL4	36 04	154	÷	-24	201	RCL4	36 04
108	RCL2	36 02	155	CHS	-22	202	RCL6	36 06
109	SIN	41	156	1	01	203	÷	-24
110	x	-35	157	+	-55	204	X ²	53
111	GSB4	23 04	158	√X	54	205	3	03
112	RCL5	36 05	159	RCL5	36 05	206	x	-35
113	PRTX	-14	160	x	-35	207	4	04
114	RCL6	36 06	161	GSB4	23 04	208	÷	-24
115	RCL2	36 02	162	RCLI	36 46	209	RTN	24
116	SIN	41	163	GSB5	23 05	210	*LBL4	21 04
117	x	-35	164	RTN	24	211	DSP4	-63 04
118	PRTX	-14	165	*LBLD	21 14	212	PRTX	-14
119	SPC	16-11	166	GSB6	23 06	213	RTN	24
120	RCL2	36 02	167	RCL4	36 04	214	*LBL5	21 05
121	GSB5	23 05	168	GSB4	23 04	215	DSP2	-63 02
122	RTN	24	169	RCL6	36 06	216	PRTX	-14

Apparent Crystal Parameters (Concluded)								
217	RTN	24	220	*LBL7	21 07	223	RTN	24
218	*LBL6	21 06	221	SPC	16-11	224	R/S	51
219	SPC	16-11	222	SPC	16-11			

Ames Research Center

National Aeronautics and Space Administration

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APPENDIX

FORMULAS FOR DETERMINING INTERPLANAR SPACINGS, INTERPLANAR ANGLES, AND INTERZONAL ANGLES

Listed below are formulas for determining interplanar spacings, interplanar angles, and interzonal angles. These formulas were originated by K. W. Andrews, D. J. Dyson, and S. R. Keown in their publication "Interpretation of Electron Diffraction Patterns," New York, 1967. For convenience, the following codes are used for each crystal system:

a designates formulas for determining interplanar spacings of the (hkl) plane

b designates formulas for determining interplanar angle ϕ between $(h_1k_1l_1)$ and $(h_2k_2l_2)$

c designates formulas for determining interzonal angle ρ between $(u_1v_1w_1)$ and $(u_2v_2w_2)$

Crystal system: Cubic

$$a = b = c$$

$$\alpha = \beta = \gamma = 90^\circ$$

$$a \quad \frac{1}{d^2} = \frac{1}{a^2} (h^2 + k^2 + l^2)$$

$$b \quad \cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}}$$

$$c \quad \cos\rho = \frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}}$$

Crystal system: Tetragonal

$$a = b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

$$a \quad \frac{1}{d^2} = \frac{1}{a^2} (h^2 + k^2) + \frac{1}{c^2} (l^2)$$

$$b \quad \cos \phi = \frac{\frac{1}{a^2} (h_1 h_2 + k_1 k_2) + \frac{1}{c^2} (l_1 l_2)}{\sqrt{\left[\frac{1}{a^2} (h_1^2 + k_1^2) + \frac{1}{c^2} l_1^2 \right] \left[\frac{1}{a^2} (h_2^2 + k_2^2) + \frac{1}{c^2} l_2^2 \right]}}$$

$$c \quad \cos \rho = \frac{a^2 (u_1 u_2 + v_1 v_2) + c^2 w_1 w_2}{\sqrt{[a^2 (u_1^2 + v_1^2) + c^2 w_1^2] [a^2 (u_2^2 + v_2^2) + c^2 w_2^2]}}$$

Crystal system: Orthorhombic

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

$$a \quad \frac{1}{d^2} = \frac{1}{a^2} (h^2) + \frac{1}{b^2} (k^2) + \frac{1}{c^2} (l^2)$$

$$b \quad \cos \phi = \frac{\frac{1}{a^2} h_1 h_2 + \frac{1}{b^2} k_1 k_2 + \frac{1}{c^2} l_1 l_2}{\sqrt{\left(\frac{1}{a^2} h_1^2 + \frac{1}{b^2} k_1^2 + \frac{1}{c^2} l_1^2 \right) \left(\frac{1}{a^2} h_2^2 + \frac{1}{b^2} k_2^2 + \frac{1}{c^2} l_2^2 \right)}}$$

$$c \quad \cos \rho = \frac{a^2 u_1 u_2 + b^2 v_1 v_2 + c^2 w_1 w_2}{\sqrt{(a^2 u_1^2 + b^2 v_1^2 + c^2 w_1^2) (a^2 u_2^2 + b^2 v_2^2 + c^2 w_2^2)}}$$

Crystal system: Hexagonal

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ; \gamma = 120^\circ$$

$$a \quad \frac{1}{d^2} = \frac{4}{3a^2} (h^2 + hk + k^2) + \frac{1}{c^2} (l^2)$$

$$b \quad \cos \phi = \frac{h_1 h_2 + k_1 k_2 + \frac{1}{2} (h_1 k_2 + k_1 h_2) + \frac{3}{4} \frac{a^2}{c^2} l_1 l_2}{\sqrt{\left(h_1^2 + k_1^2 + h_1 k_1 + \frac{3}{4} \frac{a^2}{c^2} l_1^2 \right) \left(h_2^2 + k_2^2 + h_2 k_2 + \frac{3}{4} \frac{a^2}{c^2} l_2^2 \right)}}$$

$$c \quad \cos \rho = \frac{u_1 u_2 + v_1 v_2 - \frac{1}{2} (u_1 v_2 + v_1 u_2) + \frac{c^2}{a^2} w_1 w_2}{\sqrt{\left(u_1^2 + v_1^2 - u_1 v_1 + \frac{c^2}{a^2} w_1^2 \right) \left(u_2^2 + v_2^2 - u_2 v_2 + \frac{c^2}{a^2} w_2^2 \right)}}$$

Crystal system: Rhombohedral

$$a = b = c$$

$$\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$$

$$a \quad \frac{1}{d^2} = \frac{1}{a^2} \frac{(1 + \cos\alpha) \left[(h^2 + k^2 + l^2) - \left(1 - \tan^2 \frac{1}{2} \alpha \right) (hk + kl + lh) \right]}{1 + \cos\alpha - 2 \cos^2 \alpha}$$

b Convert to corresponding hexagonal indices and use the hexagonal system formula.

c Convert to corresponding hexagonal indices and use the hexagonal system formula.

Crystal system: Monoclinic

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ \neq \beta$$

$$a \quad \frac{1}{d^2} = \frac{1}{a^2} \frac{h^2}{\sin^2 \beta} + \frac{1}{b^2} (k^2) + \frac{1}{c^2} \frac{l^2}{\sin^2 \beta} - \frac{2hl \cos \beta}{ac \sin^2 \beta}$$

$$b \quad \cos \phi = \frac{\frac{1}{a^2} h_1 h_2 + \frac{1}{b^2} k_1 k_2 \sin^2 \beta + \frac{1}{c^2} l_1 l_2 - \frac{1}{ac} (l_1 h_2 + l_2 h_1) \cos \beta}{\left(\left(\frac{1}{a^2} h_1^2 + \frac{1}{b^2} k_1^2 \sin^2 \beta + \frac{1}{c^2} l_1^2 - \frac{2h_1 l_1}{ac} \cos \beta \right) \times \right)^{1/2} \left(\frac{1}{a^2} h_2^2 + \frac{1}{b^2} k_2^2 \sin^2 \beta + \frac{1}{c^2} l_2^2 - \frac{2h_2 l_2}{ac} \cos \beta \right)^{1/2}}$$

$$c \quad \cos \rho = \frac{a^2 u_1 u_2 + b^2 v_1 v_2 + c^2 w_1 w_2 + ac(w_1 u_2 + u_1 w_2) \cos \beta}{\left((a^2 u_1^2 + b^2 v_1^2 + c^2 w_1^2 + 2acu_1 w_1 \cos \beta) \times \right)^{1/2} \left((a^2 u_2^2 + b^2 v_2^2 + c^2 w_2^2 + 2acu_2 w_2 \cos \beta) \right)^{1/2}}$$

Crystal system: Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma$$

$$a \quad \frac{1}{d^2} = \frac{1}{v^2} (s_{11} h^2 + s_{22} k^2 + s_{33} l^2 + 2s_{12} hk + 2s_{23} kl + 2s_{31} lh)$$

where $V^2 = a^2b^2c^2(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2 \cos\alpha\cos\beta\cos\gamma)$

and

$$s_{11} = b^2c^2\sin^2\alpha$$

$$s_{22} = a^2c^2\sin^2\beta$$

$$s_{33} = a^2b^2\sin^2\gamma$$

$$s_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$$

$$s_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$$

$$s_{31} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$$

$$b \quad \cos\phi = \frac{F}{A_{h_1k_1l_1} \cdot A_{h_2k_2l_2}}$$

where $F = h_1h_2b^2c^2\sin^2\alpha + k_1k_2a^2c^2\sin^2\beta + l_1l_2a^2b^2\sin^2\gamma$

$$+ abc^2(\cos\alpha\cos\beta - \cos\gamma)(k_1h_2 + h_1k_2)$$

$$+ ab^2c(\cos\gamma\cos\alpha - \cos\beta)(h_1l_2 + l_1h_2)$$

$$+ a^2bc(\cos\beta\cos\gamma - \cos\alpha)(k_1l_2 + l_1k_2)$$

and

$$A_{hkl} = \sqrt{\begin{pmatrix} h^2b^2c^2\sin^2\alpha + k^2a^2c^2\sin^2\beta + l^2a^2b^2\sin^2\gamma \\ + 2hkabc^2(\cos\alpha\cos\beta - \cos\gamma) \\ + 2hlab^2c(\cos\gamma\cos\alpha - \cos\beta) \\ + 2kla^2bc(\cos\beta\cos\gamma - \cos\alpha) \end{pmatrix}}$$

$$c \quad \cos\rho = \frac{L}{I_{u_1v_1w_1} I_{u_2v_2w_2}}$$

where

$$\begin{aligned}L &= a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2 \\ &+ bc(v_1w_2 + w_1v_2)\cos\alpha \\ &+ ac(w_1u_2 + u_1w_2)\cos\beta \\ &+ ab(u_1v_2 + v_1u_2)\cos\gamma\end{aligned}$$

and

$$I_{uvw} = \sqrt{a^2u^2 + b^2v^2 + c^2w^2 + 2bcvw \cos\alpha + 2cawu \cos\beta + 2abuv \cos\gamma}$$

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