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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 lèngths 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 referrable 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:

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

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

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

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:

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

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

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

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

The Input and output parameters are:

	Input parameters	Output parameters[a]
Label A Calculate d	Register 1- a Register 4- h Register 5- k Register 6- 1	d or d hkl h k 1
Label B Calculate a	Register 4- h Register 5- k Register 6- 1 Register D- d	a
Label C Calculate all possible d's within limits NOTE: h<k<1 Reg. 7<8<9	Register 1- a Register 7- largest h to be printed Register 8- largest k to be printed Register 9- largest 1 to be printed Register E- only d values larger than this printed	d hkl
Label D Calculate angle (ϕ) between crystal planes or Calculate angle (ρ) between crystal zones	Register 4- h_1 (u_1) Register 5- k_1 (v_1) Register 6- 1_1 (w_1) Register 7- h_2 (u_2) Register 8- k_2 (v_2) Register 9- 1_2 (w_2)	ϕ (ρ) $h_1k_1l_1$ ($u_1v_1w_1$) $h_2k_2l_2$ ($u_2v_2w_2$)	ϕ (ρ) h_1 (u_1) k_1 (v_1) 1_1 (w_1) h_2 (u_2) k_2 (v_2) 1_2 (w_2)

[a]If h, k, and 1 (u, v, and w) are zero or positive and less than 10, output is in the form hkl (uvw). If h, k, or 1 (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h \\ k \\ 1 \end{matrix}$ or $\begin{matrix} u \\ v \\ w \end{matrix}$ (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

ØØ1	*LBLA	21 11	Ø52	RCL6	36 Ø6	1Ø3	√X	54
ØØ2	GSB1	23 Ø1	Ø53	RCL5	36 Ø5	1Ø4	RCLA	36 11
ØØ3	÷	-24	Ø54	X=Y?	16-33	1Ø5	X⇌Y	-41
ØØ4	√X	54	Ø55	GTOc	22 16 13	1Ø6	÷	-24
ØØ5	DSP4	-63 Ø4	Ø56	RCL8	36 Ø8	1Ø7	COS^{-1}	16 42
ØØ6	PRTX	-14	Ø57	X=Y?	16-33	1Ø8	DSP2	-63 Ø2
ØØ7	GSB2	23 Ø2	Ø58	GTOc	22 16 13	1Ø9	PRTX	-14
ØØ8	RTN	24	Ø59	X⇌Y	-41	11Ø	GSB2	23 Ø2
ØØ9	*LBLB	21 12	Ø6Ø	1	Ø1	111	9	Ø9
Ø1Ø	SPC	16-11	Ø61	+	-55	112	RCL7	36 Ø7
Ø11	RCLD	36 14	Ø62	STO5	35 Ø5	113	X>Y?	16-34
Ø12	GSBa	23 16 11	Ø63	STO6	35 Ø6	114	GTO9	22 Ø9
Ø13	√X	54	Ø64	GTO7	22 Ø7	115	X<Ø?	16-45
Ø14	x	-35	Ø65	*LBLc	21 16 13	116	GTO9	22 Ø9
Ø15	DSP4	-63 Ø4	Ø66	RCL5	36 Ø5	117	9	Ø9
Ø16	PRTX	-14	Ø67	RCL4	36 Ø4	118	RCL8	36 Ø8
Ø17	RTN	24	Ø68	X=Y?	16-33	119	X>Y?	16-34
Ø18	*LBLC	21 13	Ø69	R/S	51	12Ø	GTO9	22 Ø9
Ø19	RCL9	36 Ø9	Ø7Ø	RCL7	36 Ø7	121	X<Ø?	16-45
Ø2Ø	RCL8	36 Ø8	Ø71	X=Y?	16-33	122	GTO9	22 Ø9
Ø21	X>Y?	16-34	Ø72	R/S	51	123	9	Ø9
Ø22	R/S	51	Ø73	X⇌Y	-41	124	RCL9	36 Ø9
Ø23	RCL7	36 Ø7	Ø74	1	Ø1	125	X>Y?	16-34
Ø24	X>Y?	16-34	Ø75	+	-55	126	GTO9	22 Ø9
Ø25	R/S	51	Ø76	STO4	35 Ø4	127	X<Ø?	16-45
Ø26	Ø	ØØ	Ø77	STO5	35 Ø5	128	GTO9	22 Ø9
Ø27	STO4	35 Ø4	Ø78	STO6	35 Ø6	129	RCL7	36 Ø7
Ø28	STO5	35 Ø5	Ø79	GTO7	22 Ø7	13Ø	1	Ø1
Ø29	STO6	35 Ø6	Ø8Ø	*LBLD	21 14	131	Ø	ØØ
Ø3Ø	*LBLØ	21 ØØ	Ø81	RCL4	36 Ø4	132	Ø	ØØ
Ø31	RCL9	36 Ø9	Ø82	RCL7	36 Ø7	133	x	-35
Ø32	RCL6	36 Ø6	Ø83	x	-35	134	+	-55
Ø33	X=Y?	16-33	Ø84	RCL5	36 Ø5	135	RCL8	36 Ø8
Ø34	GTOb	22 16 12	Ø85	RCL8	36 Ø8	136	1	Ø1
Ø35	1	Ø1	Ø86	x	-35	137	Ø	ØØ
Ø36	+	-55	Ø87	+	-55	138	x	-35
Ø37	STO6	35 Ø6	Ø88	RCL6	36 Ø6	139	+	-55
Ø38	*LBL7	21 Ø7	Ø89	RCL9	36 Ø9	14Ø	DSPØ	-63 ØØ
Ø39	GSBd	23 16 14	Ø9Ø	x	-35	141	PRTX	-14
Ø4Ø	÷	-24	Ø91	+	-55	142	RTN	24
Ø41	√X	54	Ø92	STOA	35 11	143	*LBL1	21 Ø1
Ø42	RCLE	36 15	Ø93	RCL7	36 Ø7	144	SPC	16-11
Ø43	X>Y?	16-34	Ø94	X^2	53	145	*LBLd	21 16 14
Ø44	GTOb	22 16 12	Ø95	RCL8	36 Ø8	146	RCL1	36 Ø1
Ø45	X⇌Y	-41	Ø96	X^2	53	147	X^2	53
Ø46	SPC	16-11	Ø97	+	-55	148	*LBLa	21 16 11
Ø47	DSP4	-63 Ø4	Ø98	RCL9	36 Ø9	149	RCL4	36 Ø4
Ø48	PRTX	-14	Ø99	X^2	53	15Ø	X^2	53
Ø49	GSB2	23 Ø2	100	+	-55	151	RCL5	36 Ø5
Ø5Ø	GTOØ	22 ØØ	1Ø1	GSBa	23 16 11	152	X^2	53
Ø51	*LBLb	21 16 12	1Ø2	x	-35	153	+	-55

Cubic Calculations (Concluded)

154	RCL6	36 Ø6	173	X>Y?	16-34	192	RCL4	36 Ø4
155	X^2	53	174	GTO8	22 Ø8	193	DSPØ	-63 ØØ
156	+	-55	175	X<Ø?	16-45	194	PRTX	-14
157	RTN	24	176	GTO8	22 Ø8	195	RCL5	36 Ø5
158	*LBL2	21 Ø2	177	RCL4	36 Ø4	196	PRTX	-14
159	9	Ø9	178	1	Ø1	197	RCL6	36 Ø6
16Ø	RCL4	36 Ø4	179	Ø	ØØ	198	PRTX	-14
161	X>Y?	16-34	18Ø	Ø	ØØ	199	RTN	24
162	GTO8	22 Ø8	181	x	-35	2ØØ	*LBL9	21 Ø9
163	X<Ø?	16-45	182	+	-55	2Ø1	RCL7	36 Ø7
164	GTO8	22 Ø8	183	RCL5	36 Ø5	2Ø2	DSPØ	-63 ØØ
165	9	Ø9	184	1	Ø1	2Ø3	PRTX	-14
166	RCL5	36 Ø5	185	Ø	ØØ	2Ø4	RCL8	36 Ø8
167	X>Y?	16-34	186	x	-35	2Ø5	PRTX	-14
168	GTO8	22 Ø8	187	+	-55	2Ø6	RCL9	36 Ø9
169	X<Ø?	16-45	188	DSPØ	-63 ØØ	2Ø7	PRTX	-14
17Ø	GTO8	22 Ø8	189	PRTX	-14	2Ø8	RTN	24
171	9	Ø9	19Ø	RTN	24	2Ø9	R/S	51
172	RCL6	36 Ø6	191	*LBL8	21 Ø8			

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:

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

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

$$c = ad_1l \left[\left|\frac{1}{a^2 - d^2(h^2 + k^2)}\right|\right]^{1/2}$$

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

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

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 Reg. 7<8	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 2	Register 3- c	$h_1k_1l_1$		h_1
Calculate angle	Register 4- h_1	$h_2k_2l_2$		k_1
(ϕ) between	Register 5- k_1			l_1
crystal planes	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	$u_1v_1w_1$		u_1
Calculate angle	Register 4- u_1	$u_2v_2w_2$		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			

[a] If 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 $\begin{matrix} h \\ k \\ l \end{matrix}$ or $\begin{matrix} u \\ v \\ w \end{matrix}$ (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
14Ø	RCL6	36 Ø6						

Card 2. Tetragonal

ØØ1	*LBLD	21 14	Ø48	X>Y?	16-34	Ø95	X>Y?	16-34
ØØ2	GSBe	23 16 15	Ø49	GTO7	22 Ø7	Ø96	GTO8	22 Ø8
ØØ3	÷	-24	Ø5Ø	X<Ø?	16-45	Ø97	X<Ø?	16-45
ØØ4	GSB4	23 Ø4	Ø51	GTO7	22 Ø7	Ø98	GTO8	22 Ø8
ØØ5	÷	-24	Ø52	RCL7	36 Ø7	Ø99	9	Ø9
ØØ6	+	-55	Ø53	1	Ø1	1ØØ	RCL5	36 Ø5
ØØ7	STOA	35 11	Ø54	Ø	ØØ	1Ø1	X>Y?	16-34
ØØ8	GSB2	23 Ø2	Ø55	Ø	ØØ	1Ø2	GTO8	22 Ø8
ØØ9	RCL1	36 Ø1	Ø56	x	-35	1Ø3	X<Ø?	16-45
Ø1Ø	X^2	53	Ø57	+	-55	1Ø4	GTO8	22 Ø8
Ø11	÷	-24	Ø58	RCL8	36 Ø8	1Ø5	9	Ø9
Ø12	RCL6	36 Ø6	Ø59	1	Ø1	1Ø6	RCL6	36 Ø6
Ø13	RCL3	36 Ø3	Ø6Ø	Ø	ØØ	1Ø7	X>Y?	16-34
Ø14	÷	-24	Ø61	x	-35	1Ø8	GTO8	22 Ø8
Ø15	GSB6	23 Ø6	Ø62	+	-55	1Ø9	X<Ø?	16-45
Ø16	÷	-24	Ø63	PRTX	-14	11Ø	GTO8	22 Ø8
Ø17	RCL9	36 Ø9	Ø64	RTN	24	111	RCL4	36 Ø4
Ø18	RCL3	36 Ø3	Ø65	*LBLE	21 15	112	1	Ø1
Ø19	÷	-24	Ø66	GSBe	23 16 15	113	Ø	ØØ
Ø2Ø	*LBL9	21 Ø9	Ø67	x	-35	114	Ø	ØØ
Ø21	X^2	53	Ø68	RCL6	36 Ø6	115	x	-35
Ø22	+	-55	Ø69	RCL9	36 Ø9	116	+	-55
Ø23	x	-35	Ø7Ø	x	-35	117	RCL5	36 Ø5
Ø24	$\sqrt{X}$	54	Ø71	RCL3	36 Ø3	118	1	Ø1
Ø25	RCLA	36 11	Ø72	X^2	53	119	Ø	ØØ
Ø26	X⇌Y	-41	Ø73	x	-35	12Ø	x	-35
Ø27	÷	-24	Ø74	+	-55	121	+	-55
Ø28	COS^{-1}	16 42	Ø75	STOA	35 11	122	PRTX	-14
Ø29	SPC	16-11	Ø76	GSB2	23 Ø2	123	RTN	24
Ø3Ø	FIX	-11	Ø77	RCL1	36 Ø1	124	*LBL2	21 Ø2
Ø31	DSP2	-63 Ø2	Ø78	X^2	53	125	RCL4	36 Ø4
Ø32	PRTX	-14	Ø79	x	-35	126	X^2	53
Ø33	GSB1	23 Ø1	Ø8Ø	RCL6	36 Ø6	127	RCL5	36 Ø5
Ø34	9	Ø9	Ø81	RCL3	36 Ø3	128	X^2	53
Ø35	RCL7	36 Ø7	Ø82	x	-35	129	+	-55
Ø36	X>Y?	16-34	Ø83	GSB6	23 Ø6	13Ø	RTN	24
Ø37	GTO7	22 Ø7	Ø84	x	-35	131	*LBL3	21 Ø3
Ø38	X<Ø?	16-45	Ø85	RCL9	36 Ø9	132	RCL7	36 Ø7
Ø39	GTO7	22 Ø7	Ø86	RCL3	36 Ø3	133	X^2	53
Ø4Ø	9	Ø9	Ø87	x	-35	134	RCL8	36 Ø8
Ø41	RCL8	36 Ø8	Ø88	GSB9	23 Ø9	135	X^2	53
Ø42	X>Y?	16-34	Ø89	RTN	24	136	+	-55
Ø43	GTO7	22 Ø7	Ø9Ø	*LBL1	21 Ø1	137	RTN	24
Ø44	X<Ø?	16-45	Ø91	FIX	-11	138	*LBL4	21 Ø4
Ø45	GTO7	22 Ø7	Ø92	DSPØ	-63 ØØ	139	RCL6	36 Ø6
Ø46	9	Ø9	Ø93	9	Ø9	14Ø	RCL9	36 Ø9
Ø47	RCL9	36 Ø9	Ø94	RCL4	36 Ø4	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	*LBLe	21 16	15
144	RTN	24	157	RCL9	36 Ø9	169	RCL4	36	Ø4
145	*LBL6	21 Ø6	158	PRTX	-14	17Ø	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
15Ø	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	Ø4Ø	*LBL4	21 Ø4	Ø76	*LBLe	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	Ø8Ø	STO2	35	Ø2
ØØ9	x	-35	Ø45	X^2	53	Ø81	RCL6	36	Ø6
Ø1Ø	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	Ø5Ø	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	RCLE	36 15	Ø53	RCLA	36 11	Ø89	RCL1	36	Ø1
Ø18	RCL9	36 Ø9	Ø54	x	-35	Ø9Ø	STO7	35	Ø7
Ø19	x	-35	Ø55	RCLD	36 14	Ø91	RCL2	36	Ø2
Ø2Ø	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	Ø6Ø	PRTX	-14	Ø96	STOØ	35	ØØ
Ø25	-	-45	Ø61	RTN	24	Ø97	RCLE	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	1ØØ	STOE	35	15
Ø29	RCLD	36 14	Ø65	R/S	51	1Ø1	RTN		24
Ø3Ø	x	-35	Ø66	GSBe	23 16 15	1Ø2	*LBL2	21	Ø2
Ø31	RCLE	36 15	Ø67	1	Ø1	1Ø3	RCL4	36	Ø4
Ø32	x	-35	Ø68	STOC	35 13	1Ø4	X^2		53
Ø33	FIX	-11	Ø69	GTO4	22 Ø4	1Ø5	RCL5	36	Ø5
Ø34	DSP4	-63 Ø4	Ø7Ø	*LBL9	21 Ø9	1Ø6	X^2		53
Ø35	PRTX	-14	Ø71	RCLØ	36 ØØ	1Ø7	+		-55
Ø36	STOA	35 11	Ø72	X≠Ø?	16-42	1Ø8	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:

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

$$a^2 = \frac{d_1^2 d_2^2 d_3^4 [(h_3^2 1_2^2 - h_2^2 1_3^2)(k_1^2 1_3^2 - k_3^2 1_1^2) - (k_2^2 1_3^2 - k_3^2 1_2^2)(h_3^2 1_1^2 - h_1^2 1_3^2)]}{d_3^4 1_3^2 [d_2^2 (k_2^2 1_3^2 - k_3^2 1_2^2) - d_1^2 (k_1^2 1_3^2 - k_3^2 1_1^2)] + d_1^2 d_2^2 d_3^2 [1_2^2 (k_1^2 1_3^2 - k_3^2 1_1^2) - 1_1^2 (k_2^2 1_3^2 - k_3^2 1_2^2)]}$$

$$b^2 = \frac{d_2^2 d_3^2 (k_2^2 1_3^2 - k_3^2 1_2^2)}{d_3^2 1_3^2 - d_2^2 1_2^2 + [d_2^2 d_3^2 (h_3^2 1_2^2 - h_2^2 1_3^2)/a^2]}$$

$$c^2 = \frac{d_3^2 1_3^2}{1 - (d_3^2 h_3^2/a^2) - (d_3^2 k_3^2/b^2)}$$

$$\cos\phi = \frac{h_1 h_2/a^2 + k_1 k_2/b^2 + 1_1 1_2/c^2}{[(h_1^2/a^2 + k_1^2/b^2 + 1_1^2/c^2)(h_2^2/a^2 + k_2^2/b^2 + 1_2^2/c^2)]^{1/2}}$$

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

The input and output parameters are:

	Input parameters	Output parameters[a]		
Label A	Register 1- a	d	or	d
Card 1	Register 2- b	hkl		h
Calculate d	Register 3- c			k
	Register 4- h			1
	Register 5- k			
	Register 6- 1			
Label B	Register 1- h_1	a		
Card 2	Register 2- k_1	b		
Calculate a,b,c	Register 3- 1_1	c		
	Register 4- h_2			
	Register 5- k_2			
	Register 6- 1_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 Card 1 Calculate all possible d's within limits	Register 1- a Register 2- b 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	d hkl
Label D Card 3 Calculate angle (ϕ) between crystal planes	Register 1- a Register 2- b Register 3- c Register 4- h_1 Register 5- k_1 Register 6- l_1 Register 7- h_2 Register 8- k_2 Register 9- l_2	ϕ or ϕ $h_1k_1l_1$ h_1 $h_2k_2l_2$ k_1 l_1 h_2 k_2 l_2
Label E Card 3 Calculate angle (ρ) between crystal zones	Register 1- a Register 2- b Register 3- c Register 4- u_1 Register 5- v_1 Register 6- w_1 Register 7- u_2 Register 8- v_2 Register 9- w_2	ρ or ρ $u_1v_1w_2$ u_1 $u_2v_2w_2$ v_1 w_1 u_2 v_2 w_2

[a] If h, k, and 1 (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 1 (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h \\ k \\ 1 \end{matrix}$ or $\begin{matrix} u \\ v \\ w \end{matrix}$ (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

ØØ1	*LBLA	21 11	Ø49	STO5	35 Ø5	Ø97	+	-55
ØØ2	GSB1	23 Ø1	Ø5Ø	STO6	35 Ø6	Ø98	STO4	36 Ø4
ØØ3	*LBLa	21 16 11	Ø51	STOA	35 11	Ø99	Ø	ØØ
ØØ4	SPC	16-11	Ø52	*LBLØ	21 ØØ	1ØØ	STO5	35 Ø5
ØØ5	PRTX	-14	Ø53	RCL9	36 Ø9	1Ø1	STO6	35 Ø6
ØØ6	DSPØ	-63 ØØ	Ø54	RCL6	36 Ø6	1Ø2	1	Ø1
ØØ7	9	Ø9	Ø55	X=Y?	16-33	1Ø3	STOB	35 12
ØØ8	RCL4	36 Ø4	Ø56	GTOb	22 16 12	1Ø4	GTO7	22 Ø7
ØØ9	X>Y?	16-34	Ø57	1	Ø1	1Ø5	*LBL1	21 Ø1
Ø1Ø	GTO9	22 Ø9	Ø58	+	-55	1Ø6	DSP4	-63 Ø4
Ø11	X<Ø?	16-45	Ø59	STO6	35 Ø6	1Ø7	RCL4	36 Ø4
Ø12	GTO9	22 Ø9	Ø6Ø	Ø	ØØ	1Ø8	RCL1	36 Ø1
Ø13	9	Ø9	Ø61	STOB	35 12	1Ø9	÷	-24
Ø14	RCL5	36 Ø5	Ø62	*LBL7	21 Ø7	11Ø	X^2	53
Ø15	X>Y?	16-34	Ø63	Ø	ØØ	111	RCL5	36 Ø5
Ø16	GTO9	22 Ø9	Ø64	STOA	35 11	112	RCL2	36 Ø2
Ø17	X<Ø?	16-45	Ø65	GSB1	23 Ø1	113	÷	-24
Ø18	GTO9	22-Ø9	Ø66	RCLE	36 15	114	X^2	53
Ø19	9	Ø9	Ø67	X>Y?	16-34	115	+	-55
Ø2Ø	RCL6	36 Ø6	Ø68	GTO3	22 Ø3	116	RCL6	36 Ø6
Ø21	X>Y?	16-34	Ø69	X⇌Y	-41	117	RCL3	36 Ø3
Ø22	GTO9	22 Ø9	Ø7Ø	GSBa	23 16 11	118	÷	-24
Ø23	X<Ø?	16-45	Ø71	GTOØ	22 ØØ	119	X^2	53
Ø24	GTO9	22 Ø9	Ø72	*LBLb	21 16 12	12Ø	+	-55
Ø25	RCL4	36 Ø4	Ø73	RCL6	36 Ø6	121	1/X	52
Ø26	1	Ø1	Ø74	X=Ø?	16-43	122	$\sqrt{X}$	54
Ø27	Ø	ØØ	Ø75	GTO4	22 Ø4	123	RTN	24
Ø28	Ø	ØØ	Ø76	*LBL5	21 Ø5	124	*LBL3	21 Ø3
Ø29	x	-35	Ø77	RCL8	36 Ø8	125	1	Ø1
Ø3Ø	+	-55	Ø78	RCL5	36 Ø5	126	STOA	35 11
Ø31	RCL5	36 Ø5	Ø79	X=Y?	16-33	127	GTOb	22 16 12
Ø32	1	Ø1	Ø8Ø	GTOc	22 16 13	128	*LBL4	21 Ø4
Ø33	Ø	ØØ	Ø81	1	Ø1	129	RCL9	36 Ø9
Ø34	x	-35	Ø82	+	-55	13Ø	X≠Ø?	16-42
Ø35	+	-55	Ø83	STO5	35 Ø5	131	GTOc	22 16 13
Ø36	PRTX	-14	Ø84	Ø	ØØ	132	RCLA	36 11
Ø37	RTN	24	Ø85	STO6	35 Ø6	133	X≠Ø?	16-42
Ø38	*LBL9	21 Ø9	Ø86	GTO7	22 Ø7	134	GTOc	22 16 13
Ø39	RCL4	36 Ø4	Ø87	*LBLc	21 16 13	135	GTO5	22 Ø5
Ø4Ø	PRTX	-14	Ø88	RCL5	36 Ø5	136	*LBL6	21 Ø6
Ø41	RCL5	36 Ø5	Ø89	X=Ø?	16-43	137	RCL8	36 Ø8
Ø42	PRTX	-14	Ø9Ø	GTO6	22 Ø6	138	X≠Ø?	16-42
Ø43	RCL6	36 Ø6	Ø91	*LBL8	21 Ø8	139	R/S	51
Ø44	PRTX	-14	Ø92	RCL7	36 Ø7	14Ø	RCLB	36 12
Ø45	RTN	24	Ø93	RCL4	36 Ø4	141	X≠Ø?	16-42
Ø46	*LBLC	21 13	Ø94	X=Y?	16-33	142	R/S	51
Ø47	Ø	ØØ	Ø95	R/S	51	143	GTO8	22 Ø8
Ø48	STO4	35 Ø4	Ø96	1	Ø1			

Card 2. Orthorhombic

ØØ1	*LBLB	21 12	Ø52	RCLØ	36 ØØ	1Ø3	+	-55
ØØ2	SPC	16-11	Ø53	x	-35	1Ø4	X=Ø?	16-43
ØØ3	P≓S	16-51	Ø54	RCLE	36 15	1Ø5	GTOb	22 16 12
ØØ4	Ø	ØØ	Ø55	RCLI	36 46	1Ø6	RCLC	36 13
ØØ5	STO9	35 Ø9	Ø56	x	-35	1Ø7	RCL9	36 Ø9
ØØ6	P≓S	16-51	Ø57	-	-45	1Ø8	GSB1	23 Ø1
ØØ7	DSP4	-63 Ø4	Ø58	X=Ø?	16-43	1Ø9	X=Ø?	16-43
ØØ8	GSB4	23 Ø4	Ø59	GTO7	22 Ø7	11Ø	GTOb	22 16 12
ØØ9	*LBL8	21 Ø8	Ø6Ø	X≓Y	-41	111	X≓Y	-41
Ø1Ø	RCL7	36 Ø7	Ø61	÷	-24	112	÷	-24
Ø11	RCL3	36 Ø3	Ø62	STOØ	35 ØØ	113	ABS	16 31
Ø12	GSB1	23 Ø1	Ø63	ABS	16 31	114	√X	54
Ø13	RCL1	36 Ø1	Ø64	√X	54	115	PRTX	-14
Ø14	RCL9	36 Ø9	Ø65	PRTX	-14	116	RTN	24
Ø15	GSB2	23 Ø2	Ø66	*LBLe	21 16 15	117	*LBL1	21 Ø1
Ø16	RCLA	36 11	Ø67	RCLD	36 14	118	x	-35
Ø17	RCLC	36 13	Ø68	RCLØ	36 ØØ	119	X^2	53
Ø18	GSB3	23 Ø3	Ø69	÷	-24	120	RTN	24
Ø19	STOI	35 46	Ø7Ø	RCLC	36 13	121	*LBL2	21 Ø2
Ø2Ø	RCL2	36 Ø2	Ø71	RCL9	36 Ø9	122	x	-35
Ø21	RCL9	36 Ø9	Ø72	GSB1	23 Ø1	123	X^2	53
Ø22	GSB1	23 Ø1	Ø73	+	-55	124	-	-45
Ø23	RCL8	36 Ø8	Ø74	RCLB	36 12	125	RTN	24
Ø24	RCL3	36 Ø3	Ø75	RCL6	36 Ø6	126	*LBL3	21 Ø3
Ø25	GSB2	23 Ø2	Ø76	GSB2	23 Ø2	127	x	-35
Ø26	RCLA	36 11	Ø77	X=Ø?	16-43	128	X^2	53
Ø27	RCLC	36 13	Ø78	GTOa	22 16 11	129	x	-35
Ø28	GSB3	23 Ø3	Ø79	RCLE	36 15	130	RTN	24
Ø29	STOØ	35 ØØ	Ø8Ø	X=Ø?	16-43	131	*LBLa	21 16 11
Ø3Ø	RCLB	36 12	Ø81	GTOa	22 16 11	132	GSBd	23 16 14
Ø31	RCL6	36 Ø6	Ø82	X≓Y	-41	133	GTOe	22 16 15
Ø32	GSB1	23 Ø1	Ø83	÷	-24	134	*LBLb	21 16 12
Ø33	RCLØ	36 ØØ	Ø84	STOI	35 46	135	GSBd	23 16 14
Ø34	x	-35	Ø85	ABS	16 31	136	GTOc	22 16 13
Ø35	RCLC	36 13	Ø86	√X	54	137	*LBL7	21 Ø7
Ø36	RCL9	36 Ø9	Ø87	PRTX	-14	138	GSBd	23 16 14
Ø37	GSB1	23 Ø1	Ø88	*LBLc	21 16 13	139	GTO8	22 Ø8
Ø38	RCLE	36 15	Ø89	RCL7	36 Ø7	140	*LBLd	21 16 14
Ø39	RCLØ	36 ØØ	Ø9Ø	X^2	53	141	P≓S	16-51
Ø4Ø	-	-45	Ø91	RCLØ	36 ØØ	142	6	Ø6
Ø41	x	-35	Ø92	÷	-24	143	RCL9	36 Ø9
Ø42	+	-55	Ø93	RCL8	36 Ø8	144	X=Y?	16-33
Ø43	RCLA	36 11	Ø94	X^2	53	145	R/S	51
Ø44	RCL3	36 Ø3	Ø95	RCLI	36 46	146	1	Ø1
Ø45	GSB1	23 Ø1	Ø96	÷	-24	147	+	-55
Ø46	RCLE	36 15	Ø97	+	-55	148	STO9	35 Ø9
Ø47	x	-35	Ø98	RCLC	36 13	149	P≓S	16-51
Ø48	-	-45	Ø99	X^2	53	15Ø	RCLA	36 11
Ø49	X=Ø?	16-43	1ØØ	x	-35	151	RCL1	36 Ø1
Ø5Ø	GTO7	22 Ø7	1Ø1	CHS	-22	152	RCL2	36 Ø2
Ø51	RCLD	36 14	1Ø2	1	Ø1	153	RCL3	36 Ø3

Card 2. Orthorhombic (Concluded)

154	P⇌S	16-51	175	RCL5	36 Ø5	196	RCL6	36 Ø6
155	STO1	35 Ø1	176	STO8	35 Ø8	197	GSB1	23 Ø1
156	R↓	-31	177	RCL6	36 Ø6	198	RCL4	36 Ø4
157	STO2	35 Ø2	178	STO9	35 Ø9	199	RCL9	36 Ø9
158	R↓	-31	179	P⇌S	16-51	2ØØ	GSB2	23 Ø2
159	STO3	35 Ø3	180	RCL1	36 Ø1	2Ø1	RCLB	36 12
16Ø	R↓	-31	181	RCL2	36 Ø2	2Ø2	RCLC	36 13
161	STO4	35 Ø4	182	RCL3	36 Ø3	2Ø3	GSB3	23 Ø3
162	P⇌S	16-51	183	RCL4	36 Ø4	2Ø4	STOD	35 14
163	RCLC	36 13	184	P⇌S	16-51	2Ø5	RCL5	36 Ø5
164	STOA	35 11	185	STOB	35 12	2Ø6	RCL9	36 Ø9
165	RCL7	36 Ø7	186	R↓	-31	2Ø7	GSB1	23 Ø1
166	STO1	35 Ø1	187	STO4	35 Ø4	2Ø8	RCL8	36 Ø8
167	RCL8	36 Ø8	188	R↓	-31	2Ø9	RCL6	36 Ø6
168	STO2	35 Ø2	189	STO5	35 Ø5	21Ø	GSB2	23 Ø2
169	RCL9	36 Ø9	19Ø	R↓	-31	211	RCLB	36 12
17Ø	STO3	35 Ø3	191	STO6	35 Ø6	212	RCLC	36 13
171	RCLB	36 12	192	GSB4	23 Ø4	213	GSB3	23 Ø3
172	STOC	35 13	193	RTN	24	214	STOE	35 15
173	RCL4	36 Ø4	194	*LBL4	21 Ø4	215	RTN	24
174	STO7	35 Ø7	195	RCL7	36 Ø7			

Card 3. Orthorhombic

ØØ1	*LBLD	21 14	Ø29	RCL8	36 Ø8	Ø57	RCL5	36 Ø5
ØØ2	GSB6	23 Ø6	Ø3Ø	RCL2	36 Ø2	Ø58	X>Y?	16-34
ØØ3	÷	-24	Ø31	÷	-24	Ø59	GTO9	22 Ø9
ØØ4	GSBd	23 16 14	Ø32	X^2	53	Ø6Ø	X<Ø?	16-45
ØØ5	÷	-24	Ø33	+	-55	Ø61	GTO9	22 Ø9
ØØ6	+	-55	Ø34	RCL9	36 Ø9	Ø62	9	Ø9
ØØ7	GSBe	23 16 15	Ø35	RCL3	36 Ø3	Ø63	RCL6	36 Ø6
ØØ8	÷	-24	Ø36	÷	-24	Ø64	X>Y?	16-34
ØØ9	+	-55	Ø37	*LBL5	21 Ø5	Ø65	GTO9	22 Ø9
Ø1Ø	STOØ	35 ØØ	Ø38	X^2	53	Ø66	X<Ø?	16-45
Ø11	RCL4	36 Ø4	Ø39	+	-55	Ø67	GTO9	22 Ø9
Ø12	RCL1	36 Ø1	Ø4Ø	x	-35	Ø68	RCL4	36 Ø4
Ø13	÷	-24	Ø41	$\sqrt{X}$	54	Ø69	1	Ø1
Ø14	X^2	53	Ø42	RCLØ	36 ØØ	Ø7Ø	Ø	ØØ
Ø15	RCL5	36 Ø5	Ø43	X⇌Y	-41	Ø71	Ø	ØØ
Ø16	RCL2	36 Ø2	Ø44	÷	-24	Ø72	x	-35
Ø17	÷	-24	Ø45	COS^{-1}	16 42	Ø73	+	-55
Ø18	X^2	53	Ø46	DSP2	-63 Ø2	Ø74	RCL5	36 Ø5
Ø19	+	-55	Ø47	SPC	16-11	Ø75	1	Ø1
Ø2Ø	RCL6	36 Ø6	Ø48	PRTX	-14	Ø76	Ø	ØØ
Ø21	RCL3	36 Ø3	Ø49	DSPØ	-63 ØØ	Ø77	x	-35
Ø22	÷	-24	Ø5Ø	9	Ø9	Ø78	+	-55
Ø23	X^2	53	Ø51	RCL4	36 Ø4	Ø79	PRTX	-14
Ø24	+	-55	Ø52	X>Y?	16-34	Ø8Ø	*LBL4	21 Ø4
Ø25	RCL7	36 Ø7	Ø53	GTO9	22 Ø9	Ø81	9	Ø9
Ø26	RCL1	36 Ø1	Ø54	X<Ø?	16-45	Ø82	RCL7	36 Ø7
Ø27	÷	-24	Ø55	GTO9	22 Ø9	Ø83	X>Y?	16-34
Ø28	X^2	53	Ø56	9	Ø9	Ø84	GTO2	22 Ø2

Card 3. Orthorhombic (Concluded)

Ø85	X<Ø?	16-45	119	x	-35	153	RCL1	36 Ø1
Ø86	GTO2	22 Ø2	12Ø	+	-55	154	X^2	53
Ø87	9	Ø9	121	STOØ	35 ØØ	155	RTN	24
Ø88	RCL8	36 Ø8	122	RCL4	36 Ø4	156	*LBLd	21 16 14
Ø89	X>Y?	16-34	123	RCL1	36 Ø1	157	RCL5	36 Ø5
Ø9Ø	GTO2	22 Ø2	124	x	-35	158	RCL8	36 Ø8
Ø91	X<Ø?	16-45	125	X^2	53	159	x	-35
Ø92	GTO2	22 Ø2	126	RCL5	36 Ø5	16Ø	RCL2	36 Ø2
Ø93	9	Ø9	127	RCL2	36 Ø2	161	X^2	53
Ø94	RCL9	36 Ø9	128	x	-35	162	RTN	24
Ø95	X>Y?	16-34	129	X^2	53	163	*LBLe	21 16 15
Ø96	GTO2	22 Ø2	13Ø	+	-55	164	RCL6	36 Ø6
Ø97	X<Ø?	16-45	131	RCL6	36 Ø6	165	RCL9	36 Ø9
Ø98	GTO2	22 Ø2	132	RCL3	36 Ø3	166	x	-35
Ø99	RCL7	36 Ø7	133	x	-35	167	RCL3	36 Ø3
1ØØ	1	Ø1	134	X^2	53	168	X^2	53
1Ø1	Ø	ØØ	135	+	-55	169	RTN	24
1Ø2	Ø	ØØ	136	RCL7	36 Ø7	17Ø	*LBL2	21 Ø2
1Ø3	x	-35	137	RCL1	36 Ø1	171	RCL7	36 Ø7
1Ø4	+	-55	138	x	-35	172	PRTX	-14
1Ø5	RCL8	36 Ø8	139	X^2	53	173	RCL8	36 Ø8
1Ø6	1	Ø1	140	RCL8	36 Ø8	174	PRTX	-14
1Ø7	Ø	ØØ	141	RCL2	36 Ø2	175	RCL9	36 Ø9
1Ø8	x	-35	142	x	-35	176	PRTX	-14
1Ø9	+	-55	143	X^2	53	177	RTN	24
11Ø	PRTX	-14	144	+	-55	178	*LBL9	21 Ø9
111	RTN	24	145	RCL9	36 Ø9	179	RCL4	36 Ø4
112	*LBLE	21 15	146	RCL3	36 Ø3	18Ø	PRTX	-14
113	GSB6	23 Ø6	147	x	-35	181	RCL5	36 Ø5
114	x	-35	148	GTO5	22 Ø5	182	PRTX	-14
115	GSBd	23 16 14	149	*LBL6	21 Ø6	183	RCL6	36 Ø6
116	x	-35	15Ø	RCL4	36 Ø4	184	PRTX	-14
117	+	-55	151	RCL7	36 Ø7	185	GTO4	22 Ø4
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:

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

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

$$c = l_1 d_1 \left[\left[\frac{1}{1 - \{4d_1^2(h_1^2 + h_1k_1 + k_1^2)/3a^2\}}\right]\right]^{1/2}$$

$$\cos\phi = \frac{h_1h_2 + k_1k_2 + (1/2)(h_1k_2 + k_1h_2) + (3l_1l_2a^2/4c^2)}{\{[h_1^2 + k_1^2 + h_1k_1 + (3a^2l_1^2/4c^2)][h_2^2 + k_2^2 + h_2k_2 + (3a^2l_2^2/4c^2)]\}^{1/2}}$$

$$\cos\rho = \frac{u_1u_2 + v_1v_2 - (1/2)(u_1v_2 + v_1u_2) + (w_1w_2c^2/a^2)}{\{[u_1^2 + v_1^2 - u_1v_1 + (c^2w_1^2/a^2)][u_2^2 + v_2^2 - u_2v_2 + (c^2w_2^2/a^2)]\}^{1/2}}$$

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 Reg. 7<8	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 2	Register 3- c	$h_1k_1l_1$		h_1
Calculate angle (ϕ) between crystal planes	Register 4- h_1	$h_2k_2l_2$		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	$u_1v_1w_1$		u_1
Calculate angle	Register 4- u_1	$u_2v_2w_2$		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			

[a]If h, k, and 1 (u, v, and w) are 0 or positive and less then 10, output is in the form hk1 (uvw). If h, k, or 1 (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h \\ k \\ l \end{matrix}$ or $\begin{matrix} u \\ v \\ w \end{matrix}$.

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

ØØ1	*LBLA	21 11	Ø3Ø	+	-55	Ø59	GSBØ	23 ØØ
ØØ2	GSBØ	23 ØØ	Ø31	RCL5	36 Ø5	Ø6Ø	RCLE	36 15
ØØ3	FIX	-11	Ø32	1	Ø1	Ø61	X>Y?	16-34
ØØ4	PRTX	-14	Ø33	Ø	ØØ	Ø62	GTO1	22 Ø1
ØØ5	*LBLc	21 16 13	Ø34	x	-35	Ø63	X⇌Y	-41
ØØ6	DSPØ	-63 ØØ	Ø35	+	-55	Ø64	SPC	16-11
ØØ7	9	Ø9	Ø36	PRTX	-14	Ø65	FIX	-11
ØØ8	RCL4	36 Ø4	Ø37	RTN	24	Ø66	PRTX	-14
ØØ9	X>Y?	16-34	Ø38	*LBLC	21 13	Ø67	GSBc	23 16 13
Ø1Ø	GTOa	22 16 11	Ø39	RCL8	36 Ø8	Ø68	GTO5	22 Ø5
Ø11	X<Ø?	16-45	Ø4Ø	RCL7	36 Ø7	Ø69	*LBL1	21 Ø1
Ø12	GTOa	22 16 11	Ø41	X>Y?	16-34	Ø7Ø	1	Ø1
Ø13	9	Ø9	Ø42	R/S	51	Ø71	STOA	35 11
Ø14	RCL5	36 Ø5	Ø43	Ø	ØØ	Ø72	*LBL9	21 Ø9
Ø15	X>Y?	16-34	Ø44	STOA	35 11	Ø73	RCL6	36 Ø6
Ø16	GTOa	22 16 11	Ø45	STO4	35 Ø4	Ø74	X=Ø?	16-43
Ø17	X<Ø?	16-45	Ø46	STO5	35 Ø5	Ø75	GTO2	22 Ø2
Ø18	GTOa	22 16 11	Ø47	STO6	35 Ø6	Ø76	*LBL4	21 Ø4
Ø19	9	Ø9	Ø48	*LBL5	21 Ø5	Ø77	RCL8	36 Ø8
Ø2Ø	RCL6	36 Ø6	Ø49	RCL9	36 Ø9	Ø78	RCL5	36 Ø5
Ø21	X>Y?	16-34	Ø5Ø	RCL6	36 Ø6	Ø79	X=Y?	16-33
Ø22	GTOa	22 16 11	Ø51	X=Y?	16-33	Ø8Ø	GTO8	22 Ø8
Ø23	X<Ø?	16-45	Ø52	GTO9	22 Ø9	Ø81	1	Ø1
Ø24	GTOa	22 16 11	Ø53	1	Ø1	Ø82	+	-55
Ø25	RCL4	36 Ø4	Ø54	+	-55	Ø83	STO5	35 Ø5
Ø26	1	Ø1	Ø55	STO6	35 Ø6	Ø84	Ø	ØØ
Ø27	Ø	ØØ	Ø56	*LBL6	21 Ø6	Ø85	STO6	35 Ø6
Ø28	Ø	ØØ	Ø57	Ø	ØØ	Ø86	GTO6	22 Ø6
Ø29	x	-35	Ø58	STOA	35 11	Ø87	*LBL2	21 Ø2

Card 1. Hexagonal (Concluded)

Ø88	RCLA	36 11	1Ø7	*LBLØ	21 ØØ	126	PRTX	-14
Ø89	X=Ø?	16-43	1Ø8	GSBb	23 16 12	127	RCL5	36 Ø5
Ø9Ø	GTO4	22 Ø4	1Ø9	4	Ø4	128	PRTX	-14
Ø91	*LBL8	21 Ø8	11Ø	x	-35	129	RCL6	36 Ø6
Ø92	RCL5	36 Ø5	111	3	Ø3	13Ø	PRTX	-14
Ø93	RCL4	36 Ø4	112	÷	-24	131	RTN	24
Ø94	X=Y?	16-33	113	RCL1	36 Ø1	132	*LBLb	21 16 12
Ø95	R/S	51	114	X^2	53	133	DSP4	-63 Ø4
Ø96	RCL7	36 Ø7	115	÷	-24	134	RCL4	36 Ø4
Ø97	X=Y?	16-33	116	RCL6	36 Ø6	135	X^2	53
Ø98	R/S	51	117	RCL3	36 Ø3	136	RCL4	36 Ø4
Ø99	X⇌Y	-41	118	÷	-24	137	RCL5	36 Ø5
1ØØ	1	Ø1	119	X^2	53	138	x	-35
1Ø1	+	-55	12Ø	+	-55	139	+	-55
1Ø2	STO4	35 Ø4	121	1/X	52	14Ø	RCL5	36 Ø5
1Ø3	STO5	35 Ø5	122	√X	54	141	X^2	53
1Ø4	Ø	ØØ	123	RTN	24	142	+	-55
1Ø5	STO6	35 Ø6	124	*LBLa	21 16 11	143	RTN	24
1Ø6	GTO6	22 Ø6	125	RCL4	36 Ø4			

Card 2. Hexagonal

ØØ1	*LBLD	21 14	Ø31	x	-35	Ø61	x	-35
ØØ2	GSB7	23 Ø7	Ø32	+	-55	Ø62	RTN	24
ØØ3	RCL6	36 Ø6	Ø33	GSB9	23 Ø9	Ø63	*LBL2	21 Ø2
ØØ4	RCL9	36 Ø9	Ø34	RCL3	36 Ø3	Ø64	x	-35
ØØ5	x	-35	Ø35	RCL1	36 Ø1	Ø65	ABS	16 31
ØØ6	GSB8	23 Ø8	Ø36	÷	-24	Ø66	√X	54
ØØ7	+	-55	Ø37	RCL6	36 Ø6	Ø67	RCLØ	36 ØØ
ØØ8	GSB9	23 Ø9	Ø38	x	-35	Ø68	X⇌Y	-41
ØØ9	RCL6	36 Ø6	Ø39	X^2	53	Ø69	÷	-24
Ø1Ø	X^2	53	Ø4Ø	GSBØ	23 ØØ	Ø7Ø	COS^{-1}	16 42
Ø11	GSB8	23 Ø8	Ø41	-	-45	Ø71	SPC	16-11
Ø12	GSBØ	23 ØØ	Ø42	RCL3	36 Ø3	Ø72	FIX	-11
Ø13	+	-55	Ø43	RCL1	36 Ø1	Ø73	DSP2	-63 Ø2
Ø14	RCL9	36 Ø9	Ø44	÷	-24	Ø74	PRTX	-14
Ø15	X^2	53	Ø45	RCL9	36 Ø9	Ø75	*LBLa	21 16 11
Ø16	GSB8	23 Ø8	Ø46	x	-35	Ø76	FIX	-11
Ø17	GSB6	23 Ø6	Ø47	X^2	53	Ø77	DSPØ	-63 ØØ
Ø18	+	-55	Ø48	GSB6	23 Ø6	Ø78	9	Ø9
Ø19	GSB2	23 Ø2	Ø49	-	-45	Ø79	RCL4	36 Ø4
Ø2Ø	RTN	24	Ø5Ø	GSB2	23 Ø2	Ø8Ø	X>Y?	16-34
Ø21	*LBLE	21 15	Ø51	RTN	24	Ø81	GTOb	22 16 12
Ø22	GSB7	23 Ø7	Ø52	*LBL6	21 Ø6	Ø82	X<Ø?	16-45
Ø23	CHS	-22	Ø53	RCL7	36 Ø7	Ø83	GTOb	22 16 12
Ø24	RCL6	36 Ø6	Ø54	X^2	53	Ø84	9	Ø9
Ø25	RCL9	36 Ø9	Ø55	+	-55	Ø85	RCL5	36 Ø5
Ø26	x	-35	Ø56	RCL8	36 Ø8	Ø86	X>Y?	16-34
Ø27	RCL3	36 Ø3	Ø57	X^2	53	Ø87	GTOb	22 16 12
Ø28	RCL1	36 Ø1	Ø58	+	-55	Ø88	X<Ø?	16-45
Ø29	÷	-24	Ø59	RCL7	36 Ø7	Ø89	GTOb	22 16 12
Ø3Ø	X^2	53	Ø6Ø	RCL8	36 Ø8	Ø9Ø	9	Ø9

Card 2. Hexagonal (Concluded)

Ø91	RCL6	36 Ø6	128	GTOd	22 16 14	165	2	Ø2
Ø92	X>Y?	16-34	129	9	Ø9	166	÷	-24
Ø93	GTOb	22 16 12	13Ø	RCL9	36 Ø9	167	RTN	24
Ø94	X<Ø?	16-45	131	X>Y?	16-34	168	*LBL8	21 Ø8
Ø95	GTOb	22 16 12	132	GTOd	22 16 14	169	RCL1	36 Ø1
Ø96	RCL4	36 Ø4	133	X<Ø?	16-45	17Ø	RCL3	36 Ø3
Ø97	1	Ø1	134	GTOd	22 16 14	171	÷	-24
Ø98	Ø	ØØ	135	RCL7	36 Ø7	172	X^2	53
Ø99	Ø	ØØ	136	1	Ø1	173	x	-35
1ØØ	x	-35	137	Ø	ØØ	174	3	Ø3
1Ø1	+	-55	138	Ø	ØØ	175	x	-35
1Ø2	RCL5	36 Ø5	139	x	-35	176	4	Ø4
1Ø3	1	Ø1	14Ø	+	-55	177	÷	-24
1Ø4	Ø	ØØ	141	RCL8	36 Ø8	178	RTN	24
1Ø5	x	-35	142	1	Ø1	179	*LBL9	21 Ø9
1Ø6	+	-55	143	Ø	ØØ	18Ø	RCL5	36 Ø5
1Ø7	PRTX	-14	144	x	-35	181	RCL8	36 Ø8
1Ø8	GTOc	22 16 13	145	+	-55	182	x	-35
1Ø9	*LBLb	21 16 12	146	PRTX	-14	183	+	-55
11Ø	RCL4	36 Ø4	147	RTN	24	184	RCL4	36 Ø4
111	PRTX	-14	148	*LBLd	21 16 14	185	RCL7	36 Ø7
112	RCL5	36 Ø5	149	RCL7	36 Ø7	186	x	-35
113	PRTX	-14	15Ø	PRTX	-14	187	+	-55
114	RCL6	36 Ø6	151	RCL8	36 Ø8	188	STOØ	35 ØØ
115	PRTX	-14	152	PRTX	-14	189	RTN	24
116	*LBLc	21 16 13	153	RCL9	36 Ø9	19Ø	*LBLØ	21 ØØ
117	9	Ø9	154	PRTX	-14	191	RCL4	36 Ø4
118	RCL7	36 Ø7	155	RTN	24	192	X^2	53
119	X>Y?	16-34	156	*LBL7	21 Ø7	193	+	-55
12Ø	GTOd	22 16 14	157	DSP4	-63 Ø4	194	RCL5	36 Ø5
121	X<Ø?	16-45	158	RCL4	36 Ø4	195	X^2	53
122	GTOd	22 16 14	159	RCL8	36 Ø8	196	+	-55
123	9	Ø9	16Ø	x	-35	197	RCL4	36 Ø4
124	RCL8	36 Ø8	161	RCL5	36 Ø5	198	RCL5	36 Ø5
125	X>Y?	16-34	162	RCL7	36 Ø7	199	x	-35
126	GTOd	22 16 14	163	x	-35	2ØØ	RTN	24
127	X<Ø?	16-45	164	+	-55			

Card 3. Hexagonal

ØØ1	*LBLB	21 12	Ø13	X^2	53	Ø25	RCL6	36 Ø6
ØØ2	Ø	ØØ	Ø14	+	-55	Ø26	RCLD	36 14
ØØ3	STOA	35 11	Ø15	RCL6	36 Ø6	Ø27	x	-35
ØØ4	STOC	35 13	Ø16	X^2	53	Ø28	X^2	53
ØØ5	*LBL8	21 Ø8	Ø17	x	-35	Ø29	RCL9	36 Ø9
ØØ6	RCL7	36 Ø7	Ø18	GSBb	23 16 12	Ø3Ø	RCLE	36 15
ØØ7	X^2	53	Ø19	RCL9	36 Ø9	Ø31	x	-35
ØØ8	RCL7	36 Ø7	Ø2Ø	X^2	53	Ø32	X^2	53
ØØ9	RCL8	36 Ø8	Ø21	x	-35	Ø33	-	-45
Ø1Ø	x	-35	Ø22	-	-45	Ø34	3	Ø3
Ø11	+	-55	Ø23	X=Ø?	16-43	Ø35	x	-35
Ø12	RCL8	36 Ø8	Ø24	GTO6	22 Ø6	Ø36	÷	-24

Card 3. Hexagonal (Concluded)

Ø37	ABS	16 31	Ø69	GTO7	22 Ø7	1Ø1	RCL8	36 Ø8
Ø38	√X	54	Ø7Ø	1/X	52	1Ø2	STO5	35 Ø5
Ø39	2	Ø2	Ø71	ABS	16 31	1Ø3	RCL9	36 Ø9
Ø4Ø	x	-35	Ø72	√X	54	1Ø4	STO6	35 Ø6
Ø41	RCLD	36 14	Ø73	RCL6	36 Ø6	1Ø5	RCL1	36 Ø1
Ø42	x	-35	Ø74	x	-35	1Ø6	STO7	35 Ø7
Ø43	RCLE	36 15	Ø75	RCLD	36 14	1Ø7	RCL2	36 Ø2
Ø44	x	-35	Ø76	x	-35	1Ø8	STO8	35 Ø8
Ø45	STOØ	35 ØØ	Ø77	FIX	-11	1Ø9	RCL3	36 Ø3
Ø46	SPC	16-11	Ø78	PRTX	-14	110	STO9	35 Ø9
Ø47	FIX	-11	Ø79	RTN	24	111	RCLD	36 14
Ø48	DSP4	-63 Ø4	Ø8Ø	*LBLb	21 16 12	112	STOA	35 11
Ø49	PRTX	-14	Ø81	DSP4	-63 Ø4	113	RCLE	36 15
Ø5Ø	*LBL9	21 Ø9	Ø82	RCL4	36 Ø4	114	STOD	35 14
Ø51	RCL6	36 Ø6	Ø83	X^2	53	115	RCLA	36 11
Ø52	x=Ø?	16-43	Ø84	RCL4	36 Ø4	116	STOE	35 15
Ø53	GTO7	22 Ø7	Ø85	RCL5	36 Ø5	117	RTN	24
Ø54	GSBb	23 16 12	Ø86	x	-35	118	*LBL6	21 Ø6
Ø55	RCLD	36 14	Ø87	+	-55	119	RCLA	36 11
Ø56	X^2	53	Ø88	RCL5	36 Ø5	12Ø	X≠Ø?	16-42
Ø57	x	-35	Ø89	X^2	53	121	R/S	51
Ø58	4	Ø4	Ø9Ø	+	-55	122	GSBe	23 16 15
Ø59	x	-35	Ø91	RTN	24	123	GTO8	22 Ø8
Ø6Ø	3	Ø3	Ø92	*LBLe	21 16 15	124	*LBL7	21 Ø7
Ø61	÷	-24	Ø93	RCL4	36 Ø4	125	RCLC	36 13
Ø62	RCLØ	36 ØØ	Ø94	STO1	35 Ø1	126	X≠Ø?	16-42
Ø63	X^2	53	Ø95	RCL5	36 Ø5	127	R/S	51
Ø64	÷	-24	Ø96	STO2	35 Ø2	128	GSBe	23 16 15
Ø65	CHS	-22	Ø97	RCL6	36 Ø6	129	1	Ø1
Ø66	1	Ø1	Ø98	STO3	35 Ø3	13Ø	STOC	35 13
Ø67	+	-55	Ø99	RCL7	36 Ø7	131	GTO9	22 Ø9
Ø68	X=Ø?	16-43	1ØØ	STO4	35 Ø4	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:

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

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

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

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

where $H_1 = h_1 - l_1$ $K_1 = k_1 - h_1$ $L_1 = h_1 + k_1 + l_1$

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

and

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

where $U_1 = u_1 - w_1$ $V_1 = v_1 - u_1$ $W_1 = u_1 + v_1 + w_1$

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

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		h
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	Output parameters[a]		
	Register D- d_1 Register E- d_2			
Label C Card 1 Calculate all possible d's within limits NOTE: h < k < l Reg. 7 < 8 < 9	Register 1- a Register 7- largest h to be printed Register 8- largest k to be printed Register 9- largest l to be printed Register A- α Register E- only d values larger than this printed	d hkl	or	d h k l
Label D Card 2 Calculate angle (ϕ) between crystal planes	Register 1- a Register 4- h_1 Register 5- k_1 Register 6- l_1 Register 7- h_2 Register 8- k_2 Register 9- l_2 Register A- α	ϕ $h_1k_1l_1$ h_2 k_2 l_2	or	ϕ h_1 k_1 l_1 h_2 k_2 l_2
Label E Card 2 Calculate angle (ρ) between crystal zones	Register 1- a Register 4- u_1 Register 5- v_1 Register 6- w_1 Register 7- u_2 Register 8- v_2 Register 9- w_2 Register A- α	ρ $u_1v_1w_1$ u_2 v_2 w_2	or	ρ u_1 v_1 w_1 u_2 v_2 w_2

[a] If 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 $\begin{matrix} h \\ k \\ l \end{matrix}$ or $\begin{matrix} u \\ v \\ w \end{matrix}$.

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

ØØ1	*LBLA	21 11	ØØ6	PRTX	-14	Ø11	GTOb	22 16 12
ØØ2	GSB1	23 Ø1	ØØ7	DSPØ	-63 ØØ	Ø12	X<Ø?	16-45
ØØ3	*LBLa	21 16 11	ØØ8	9	Ø9	Ø13	GTOb	22 16 12
ØØ4	SPC	16-11	ØØ9	RCL4	36 Ø4	Ø14	9	Ø9
ØØ5	DSP4	-63 Ø4	Ø1Ø	X>Y?	16-34	Ø15	RCL5	36 Ø5

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	12Ø	GTOØ	22 ØØ
Ø19	GTOb	22 16 12	Ø7Ø	GTOØ	22 ØØ	121	*LBLc	21 16 13
Ø2Ø	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⇌Y	-41	129	STO6	35 Ø6
Ø28	Ø	ØØ	Ø79	GSBa	23 16 11	13Ø	GTO7	22 Ø7
Ø29	Ø	ØØ	Ø8Ø	*LBL3	21 Ø3	131	*LBLd	21 16 14
Ø3Ø	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	14Ø	STO6	35 Ø6
Ø39	*LBLC	21 13	Ø9Ø	GTO9	22 Ø9	141	GTO7	22 Ø7
Ø4Ø	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⇌Y	-41	148	PRTX	-14
Ø47	Ø	ØØ	Ø98	GSBa	23 16 11	149	RTN	24
Ø48	STO4	35 Ø4	Ø99	*LBL4	21 Ø4	15Ø	*LBL1	21 Ø1
Ø49	STO5	35 Ø5	1ØØ	RCL5	36 Ø5	151	RCL4	36 Ø4
Ø5Ø	STO6	35 Ø6	1Ø1	CHS	-22	152	X^2	53
Ø51	*LBLØ	21 ØØ	1Ø2	STO5	35 Ø5	153	RCL5	36 Ø5
Ø52	RCL9	36 Ø9	1Ø3	*LBL9	21 Ø9	154	X^2	53
Ø53	RCL6	36 Ø6	1Ø4	RCL5	36 Ø5	155	+	-55
Ø54	X=Y?	16-33	1Ø5	RCL4	36 Ø4	156	RCL6	36 Ø6
Ø55	GTOc	22 16 13	1Ø6	X=Y?	16-33	157	X^2	53
Ø56	1	Ø1	1Ø7	GTOØ	22 ØØ	158	+	-55
Ø57	ST+6	35-55 Ø6	1Ø8	CHS	-22	159	RCL4	36 Ø4
Ø58	*LBL7	21 Ø7	1Ø9	STO4	35 Ø4	16Ø	RCL5	36 Ø5
Ø59	GSB1	23 Ø1	11Ø	GSB1	23 Ø1	161	x	-35
Ø6Ø	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⇌Y	-41	114	X⇌Y	-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
17Ø	RCLA	36 11	182	1	Ø1	193	COS	42
171	2	Ø2	183	+	-55	194	X^2	53
172	÷	-24	184	x	-35	195	2	Ø2
173	TAN	43	185	RCL1	36 Ø1	196	x	-35
174	X^2	53	186	X^2	53	197	-	-45
175	CHS	-22	187	÷	-24	198	÷	-24
176	1	Ø1	188	RCLA	36 11	199	1/X	52
177	+	-55	189	COS	42	2ØØ	ABS	16 31
178	x	-35	19Ø	1	Ø1	2Ø1	$\sqrt{X}$	54
179	-	-45	191	+	-55	2Ø2	RTN	24
18Ø	RCLA	36 11						

Card 2. Rhombohedral

ØØ1	*LBLD	21 14	Ø38	X^2	53	Ø75	X>Y?	16-34
ØØ2	GSBB	23 12	Ø39	GSBØ	23 ØØ	Ø76	GTOa	22 16 11
ØØ3	RCLD	36 14	Ø4Ø	-	-45	Ø77	X<Ø?	16-45
ØØ4	RCLI	36 46	Ø41	RCL3	36 Ø3	Ø78	GTOa	22 16 11
ØØ5	x	-35	Ø42	RCL2	36 Ø2	Ø79	9	Ø9
ØØ6	GSB8	23 Ø8	Ø43	÷	-24	Ø8Ø	RCL6	36 Ø6
ØØ7	+	-55	Ø44	RCLI	36 46	Ø81	X>Y?	16-34
ØØ8	GSB9	23 Ø9	Ø45	x	-35	Ø82	GTOa	22 16 11
ØØ9	RCLD	36 14	Ø46	X^2	53	Ø83	X<Ø?	16-45
Ø1Ø	X^2	53	Ø47	GSB6	23 Ø6	Ø84	GTOa	22 16 11
Ø11	GSB8	23 Ø8	Ø48	-	-45	Ø85	RCL4	36 Ø4
Ø12	GSBØ	23 ØØ	Ø49	*LBL2	21 Ø2	Ø86	1	Ø1
Ø13	+	-55	Ø5Ø	x	-35	Ø87	Ø	ØØ
Ø14	RCLI	36 46	Ø51	ABS	16 31	Ø88	Ø	ØØ
Ø15	X^2	53	Ø52	$\sqrt{X}$	54	Ø89	GSB7	23 Ø7
Ø16	GSB8	23 Ø8	Ø53	P⇌S	16-51	Ø9Ø	RCL5	36 Ø5
Ø17	GSB6	23 Ø6	Ø54	RCLØ	36 ØØ	Ø91	1	Ø1
Ø18	+	-55	Ø55	P⇌S	16-51	Ø92	Ø	ØØ
Ø19	GSB2	23 Ø2	Ø56	X⇌Y	-41	Ø93	GSB7	23 Ø7
Ø2Ø	RTN	24	Ø57	÷	-24	Ø94	PRTX	-14
Ø21	*LBLE	21 15	Ø58	COS^{-1}	16 42	Ø95	GTOb	22 16 12
Ø22	GSBB	23 12	Ø59	SPC	16-11	Ø96	*LBLa	21 16 11
Ø23	CHS	-22	Ø6Ø	9	Ø9	Ø97	RCL4	36 Ø4
Ø24	RCLD	36 14	Ø61	Ø	ØØ	Ø98	PRTX	-14
Ø25	RCLI	36 46	Ø62	X⇌Y	-41	Ø99	RCL5	36 Ø5
Ø26	x	-35	Ø63	X>Y?	16-34	1ØØ	PRTX	-14
Ø27	RCL3	36 Ø3	Ø64	GSB5	23 Ø5	1Ø1	RCL6	36 Ø6
Ø28	RCL2	36 Ø2	Ø65	DSP2	-63 Ø2	1Ø2	PRTX	-14
Ø29	÷	-24	Ø66	PRTX	-14	1Ø3	*LBLb	21 16 12
Ø3Ø	X^2	53	Ø67	9	Ø9	1Ø4	RCL7	36 Ø7
Ø31	GSB7	23 Ø7	Ø68	RCL4	36 Ø4	1Ø5	PRTX	-14
Ø32	GSB9	23 Ø9	Ø69	X>Y?	16-34	1Ø6	RCL8	36 Ø8
Ø33	RCL3	36 Ø3	Ø7Ø	GTOa	22 16 11	1Ø7	PRTX	-14
Ø34	RCL2	36 Ø2	Ø71	X<Ø?	16-45	1Ø8	RCL9	36 Ø9
Ø35	÷	-24	Ø72	GTOa	22 16 11	1Ø9	PRTX	-14
Ø36	RCLD	36 14	Ø73	9	Ø9	11Ø	RTN	24
Ø37	x	-35	Ø74	RCL5	36 Ø5	111	*LBL6	21 Ø6

Card 2. Rhombohedral (Concluded)

112	RCLE	36 15	15Ø	+	-55	188	STOC	35 13
113	X^2	53	151	RCLB	36 12	189	RCL8	36 Ø8
114	+	-55	152	RCLC	36 13	19Ø	RCL7	36 Ø7
115	RCLØ	36 ØØ	153	x	-35	191	-	-45
116	X^2	53	154	RTN	24	192	STOØ	35 ØØ
117	+	-55	155	*LBLB	21 12	193	RCL4	36 Ø4
118	RCLE	36 15	156	RCLA	36 11	194	RCL5	36 Ø5
119	RCLØ	36 ØØ	157	2	Ø2	195	+	-55
12Ø	x	-35	158	÷	-24	196	RCL6	36 Ø6
121	RTN	24	159	SIN	41	197	+	-55
122	*LBL8	21 Ø8	16Ø	RCL1	36 Ø1	198	STOD	35 14
123	RCL2	36 Ø2	161	x	-35	199	RCL7	36 Ø7
124	RCL3	36 Ø3	162	2	Ø2	2ØØ	RCL8	36 Ø8
125	÷	-24	163	x	-35	2Ø1	+	-55
126	X^2	53	164	STO2	35 Ø2	2Ø2	RCL9	36 Ø9
127	x	-35	165	RCL1	36 Ø1	2Ø3	+	-55
128	3	Ø3	166	X^2	53	2Ø4	STOI	35 46
129	x	-35	167	9	Ø9	2Ø5	RCLB	36 12
13Ø	4	Ø4	168	x	-35	2Ø6	RCLØ	36 ØØ
131	÷	-24	169	RCL2	36 Ø2	2Ø7	x	-35
132	RTN	24	17Ø	X^2	53	2Ø8	RCLC	36 13
133	*LBL9	21 Ø9	171	3	Ø3	2Ø9	RCLE	36 15
134	RCLC	36 13	172	x	-35	21Ø	GSB7	23 Ø7
135	RCLØ	36 ØØ	173	-	-45	211	2	Ø2
136	GSB7	23 Ø7	174	ABS	16 31	212	÷	-24
137	RCLB	36 12	175	√X	54	213	RTN	24
138	RCLE	36 15	176	STO3	35 Ø3	214	*LBL5	21 Ø5
139	GSB7	23 Ø7	177	RCL4	36 Ø4	215	1	Ø1
14Ø	P⇌S	16-51	178	RCL6	36 Ø6	216	8	Ø8
141	STOØ	35 ØØ	179	-	-45	217	Ø	ØØ
142	P⇌S	16-51	18Ø	STOB	35 12	218	X⇌Y	-41
143	RTN	24	181	RCL7	36 Ø7	219	-	-45
144	*LBLØ	21 ØØ	182	RCL9	36 Ø9	22Ø	RTN	24
145	RCLB	36 12	183	-	-45	221	*LBL7	21 Ø7
146	X^2	53	184	STOE	35 15	222	x	-35
147	+	-55	185	RCL5	36 Ø5	223	+	-55
148	RCLC	36 13	186	RCL4	36 Ø4	224	RTN	24
149	X^2	53	187	-	-45			

Card 3. Rhombohedral

ØØ1	*LBLB	21 12	Ø12	RCL5	36 Ø5	Ø23	RCL7	36 Ø7
ØØ2	RCL4	36 Ø4	Ø13	x	-35	Ø24	X^2	53
ØØ3	X^2	53	Ø14	RCL5	36 Ø5	Ø25	RCL8	36 Ø8
ØØ4	RCL5	36 Ø5	Ø15	RCL6	36 Ø6	Ø26	X^2	53
ØØ5	X^2	53	Ø16	x	-35	Ø27	+	-55
ØØ6	+	-55	Ø17	+	-55	Ø28	RCL9	36 Ø9
ØØ7	RCL6	36 Ø6	Ø18	RCL6	36 Ø6	Ø29	X^2	53
ØØ8	X^2	53	Ø19	RCL4	36 Ø4	Ø3Ø	+	-55
ØØ9	+	-55	Ø2Ø	x	-35	Ø31	STO2	35 Ø2
Ø1Ø	STOØ	35 ØØ	Ø21	+	-55	Ø32	RCL7	36 Ø7
Ø11	RCL4	36 Ø4	Ø22	STO1	35 Ø1	Ø33	RCL8	36 Ø8

Card 3. Rhombohedral (Concluded)

Ø34	x	-35	Ø71	9	Ø9	1Ø7	ABS	16 31
Ø35	RCL8	36 Ø8	Ø72	Ø	ØØ	1Ø8	√X	54
Ø36	RCL9	36 Ø9	Ø73	X⇌Y	-41	1Ø9	SPC	16-11
Ø37	x	-35	Ø74	X>Y?	16-34	11Ø	FIX	-11
Ø38	+	-55	Ø75	GSB1	23 Ø1	111	DSP4	-63 Ø4
Ø39	RCL9	36 Ø9	Ø76	STOA	35 11	112	PRTX	-14
Ø4Ø	RCL7	36 Ø7	Ø77	RCLØ	36 ØØ	113	RCLA	36 11
Ø41	x	-35	Ø78	RCLA	36 11	114	DSP2	-63 Ø2
Ø42	+	-55	Ø79	COS	42	115	PRTX	-14
Ø43	STO3	35 Ø3	Ø8Ø	x	-35	116	RTN	24
Ø44	RCLE	36 15	Ø81	RCLØ	36 ØØ	117	*LBL1	21 Ø1
Ø45	X^2	53	Ø82	+	-55	118	1	Ø1
Ø46	RCL2	36 Ø2	Ø83	RCL1	36 Ø1	119	8	Ø8
Ø47	x	-35	Ø84	RCLA	36 11	12Ø	Ø	ØØ
Ø48	RCLD	36 14	Ø85	COS	42	121	X⇌Y	-41
Ø49	X^2	53	Ø86	x	-35	122	-	-45
Ø5Ø	RCLØ	36 ØØ	Ø87	2	Ø2	123	RTN	24
Ø51	x	-35	Ø88	x	-35	124	*LBLa	21 16 11
Ø52	-	-45	Ø89	-	-45	125	RCL2	36 Ø2
Ø53	STOB	35 12	Ø9Ø	RCLD	36 14	126	RCLA	36 11
Ø54	CHS	-22	Ø91	X^2	53	127	COS	42
Ø55	RCLE	36 15	Ø92	x	-35	128	x	-35
Ø56	X^2	53	Ø93	X=Ø?	16-43	129	RCL2	36 Ø2
Ø57	RCL3	36 Ø3	Ø94	GTOa	22 16 11	13Ø	+	-55
Ø58	x	-35	Ø95	*LBL2	21 Ø2	131	RCL3	36 Ø3
Ø59	RCLD	36 14	Ø96	RCLA	36 11	132	RCLA	36 11
Ø6Ø	X^2	53	Ø97	COS	42	133	COS	42
Ø61	RCL1	36 Ø1	Ø98	1	Ø1	134	x	-35
Ø62	x	-35	Ø99	+	-55	135	2	Ø2
Ø63	-	-45	1ØØ	RCLA	36 11	136	x	-35
Ø64	2	Ø2	1Ø1	COS	42	137	-	-45
Ø65	x	-35	1Ø2	X^2	53	138	RCLE	36 15
Ø66	+	-55	1Ø3	2	Ø2	139	X^2	53
Ø67	RCLB	36 12	1Ø4	x	-35	14Ø	x	-35
Ø68	X⇌Y	-41	1Ø5	-	-45	141	GTO2	22 Ø2
Ø69	÷	-24	1Ø6	÷	-24	142	R/S	51
Ø7Ø	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:

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

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

$$h_H = h_R - 1_R$$

$$k_H = k_R - h_R$$

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

$$1_H = h_R + k_R + 1_R$$

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

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

$$h_R = \frac{h_H - k_H + 1_H}{3}$$

$$k_R = \frac{h_H + 2k_H + 1_H}{3}$$

$$1_R = \frac{-2h_H - k_H + 1_H}{3}$$

The input and output parameters are:

	Input parameters	Output parameters
Label A Calculate a_H, c_H	Register 1- a_R Register A- α_R	a_H c_H
Label B[a] Calculate $h_H k_H . 1_H$	Register 4- h_R Register 5- k_R Register 6- 1_R	$h_H k_H . 1_H$ or h_H k_H 1_H
Label C Calculate a_R, α_R	Register 1- a_H Register 3- c_H	a_R α_R
Label D[a] Calculate $h_R k_R 1_R$	Register 4- h_H Register 5- k_H Register 6- 1_H	$h_R k_R 1_R$ or h_R k_R 1_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

[a] If h, k, and 1 are 0, or positive integers less than 10, output is in the form hk1 or hk.1. If h, k, or 1 are negative, greater than 9, or not integers, output is in the form $\begin{matrix} h \\ k \\ 1 \end{matrix}$.

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 ⇌ Rhombohedral Calculations

ØØ1	*LBLA	21 11	Ø34	X<Ø?	16-45	Ø67	PRTX	-14
ØØ2	RCLA	36 11	Ø35	GTOa	22 16 11	Ø68	RCLD	36 14
ØØ3	2	Ø2	Ø36	9	Ø9	Ø69	PRTX	-14
ØØ4	÷	-24	Ø37	RCLC	36 13	Ø7Ø	RTN	24
ØØ5	SIN	41	Ø38	X>Y?	16-34	Ø71	*LBLC	21 13
ØØ6	RCL1	36 Ø1	Ø39	GTOa	22 16 11	Ø72	RCL1	36 Ø1
ØØ7	x	-35	Ø4Ø	X<Ø?	16-45	Ø73	X^2	53
ØØ8	2	Ø2	Ø41	GTOa	22 16 11	Ø74	3	Ø3
ØØ9	x	-35	Ø42	9	Ø9	Ø75	÷	-24
Ø1Ø	SPC	16-11	Ø43	RCLD	36 14	Ø76	RCL3	36 Ø3
Ø11	DSP4	-63 Ø4	Ø44	X>Y?	16-34	Ø77	X^2	53
Ø12	PRTX	-14	Ø45	GTOa	22 16 11	Ø78	9	Ø9
Ø13	STOØ	35 ØØ	Ø46	X<Ø?	16-45	Ø79	÷	-24
Ø14	RCL1	36 Ø1	Ø47	GTOa	22 16 11	Ø8Ø	+	-55
Ø15	X^2	53	Ø48	DSP1	-63 Ø1	Ø81	√X	54
Ø16	9	Ø9	Ø49	RCLB	36 12	Ø82	SPC	16-11
Ø17	x	-35	Ø5Ø	1	Ø1	Ø83	DSP4	-63 Ø4
Ø18	RCLØ	36 ØØ	Ø51	Ø	ØØ	Ø84	PRTX	-14
Ø19	X^2	53	Ø52	x	-35	Ø85	RCL3	36 Ø3
Ø2Ø	3	Ø3	Ø53	RCLC	36 13	Ø86	RCL1	36 Ø1
Ø21	x	-35	Ø54	+	-55	Ø87	÷	-24
Ø22	-	-45	Ø55	RCLD	36 14	Ø88	X^2	53
Ø23	ABS	16 31	Ø56	1	Ø1	Ø89	3	Ø3
Ø24	√X	54	Ø57	Ø	ØØ	Ø9Ø	+	-55
Ø25	PRTX	-14	Ø58	÷	-24	Ø91	√X	54
Ø26	RTN	24	Ø59	+	-55	Ø92	2	Ø2
Ø27	*LBLB	21 12	Ø6Ø	PRTX	-14	Ø93	x	-35
Ø28	GSB2	23 Ø2	Ø61	RTN	24	Ø94	3	Ø3
Ø29	SPC	16-11	Ø62	*LBLa	21 16 11	Ø95	X⇌Y	-41
Ø3Ø	9	Ø9	Ø63	DSPØ	-63 ØØ	Ø96	÷	-24
Ø31	RCLB	36 12	Ø64	RCLB	36 12	Ø97	SIN^{-1}	16-41
Ø32	X>Y?	16-34	Ø65	PRTX	-14	Ø98	2	Ø2
Ø33	GTOa	22 16 11	Ø66	RCLC	36 13	Ø99	x	-35

Hexagonal ⇌ Rhombohedral Calculations (Concluded)

1ØØ	DSP2	-63 Ø2	137	GTOa	22 16 11	174	PRTX	-14
1Ø1	PRTX	-14	138	X<Ø?	16-45	175	RTN	24
1Ø2	RTN	24	139	GTOa	22 16 11	176	*LBLE	21 15
1Ø3	*LBLD	21 14	14Ø	FRC	16 44	177	GSB2	23 Ø2
1Ø4	RCL4	36 Ø4	141	X≠Ø?	16-42	178	RCLB	36 12
1Ø5	RCL5	36 Ø5	142	GTOa	22 16 11	179	RCLC	36 13
1Ø6	-	-45	143	9	Ø9	18Ø	+	-55
1Ø7	RCL6	36 Ø6	144	RCLC	36 13	181	CHS	-22
1Ø8	+	-55	145	X>Y?	16-34	182	STOE	36 15
1Ø9	3	Ø3	146	GTOa	22 16 11	183	DSPØ	-63 ØØ
11Ø	÷	-24	147	X<Ø?	16-45	184	SPC	16-11
111	STOB	35 12	148	GTOa	22 16 11	185	RCLB	36 12
112	RCL4	36 Ø4	149	FRC	16 44	186	PRTX	-14
113	RCL5	36 Ø5	15Ø	X≠Ø?	16-42	187	RCLC	36 13
114	2	Ø2	151	GTOa	22 16 11	188	PRTX	-14
115	x	-35	152	9	Ø9	189	RCLE	36 15
116	+	-55	153	RCLD	36 14	19Ø	PRTX	-14
117	RCL6	36 Ø6	154	X>Y?	16-34	191	RCLD	36 14
118	+	-55	155	GTOa	22 16 11	192	PRTX	-14
119	3	Ø3	156	X<Ø?	16-45	193	RTN	24
12Ø	÷	-24	157	GTOa	22 16 11	194	*LBL2	21 Ø2
121	STOC	35 13	158	FRC	16 44	195	RCL4	36 Ø4
122	RCL4	36 Ø4	159	X≠Ø?	16-42	196	RCL6	36 Ø6
123	2	Ø2	16Ø	GTOa	22 16 11	197	-	-45
124	x	-35	161	RCLB	36 12	198	STOB	35 12
125	CHS	-22	162	1	Ø1	199	RCL5	36 Ø5
126	RCL5	36 Ø5	163	Ø	ØØ	2ØØ	RCL4	36 Ø4
127	-	-45	164	Ø	ØØ	2Ø1	-	-45
128	RCL6	36 Ø6	165	x	-35	2Ø2	STOC	35 13
129	+	-55	166	RCLC	36 13	2Ø3	RCL4	36 Ø4
13Ø	3	Ø3	167	1	Ø1	2Ø4	RCL5	36 Ø5
131	÷	-24	168	Ø	ØØ	2Ø5	+	-55
132	STOD	35 14	169	x	-35	2Ø6	RCL6	36 Ø6
133	SPC	16-11	17Ø	+	-55	2Ø7	+	-55
134	9	Ø9	171	RCLD	36 14	2Ø8	STOD	35 14
135	RCLB	36 12	172	+	-55	2Ø9	RTN	24
136	X>Y?	16-34	173	DSPØ	-63 ØØ	21Ø	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:

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

$$\cos\phi = \frac{h_1h_2/a^2 + k_1k_2\sin^2\beta/b^2 + l_1l_2/c^2 - (l_1h_2 + l_2h_1)\cos\beta/ac}{\left((h_1^2/a^2 + k_1^2\sin^2\beta/b^2 + l_1^2/c^2 - 2h_1l_1\cos\beta/ac)^{1/2} \times (h_2^2/a^2 + k_2^2\sin^2\beta/b^2 + l_2^2/c^2 - 2h_2l_2\cos\beta/ac)^{1/2}\right)}$$

$$\cos\rho = \frac{a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2 + ac(w_1u_2 + u_1w_2)\cos\beta}{\left((a^2u_1^2 + b^2v_1^2 + c^2w_1^2 + 2acu_1w_1\cos\beta)^{1/2} \times (a^2u_2^2 + b^2v_2^2 + c^2w_2^2 + 2acu_2w_2\cos\beta)^{1/2}\right)}$$

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	Register 3- c			k
possible d's	Register 7- largest h			l
within limits	to be printed			
	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	$h_1k_1l_1$		h_1
Calculate angle	Register 3- c	$h_2k_2l_2$		k_1
(ϕ) between	Register 4- h_1			l_1
crystal planes	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	$u_1v_1w_1$ u_1
Calculate angle	Register 3- c	$u_2v_2w_2$ 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	

[a]If 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 $\begin{matrix} h \\ k \\ l \end{matrix}$ or $\begin{matrix} u \\ v \\ w \end{matrix}$.

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

ØØ1	*LBLA	21 11	Ø29	Ø	ØØ	Ø57	GSBD	23 14
ØØ2	GSB1	23 Ø1	Ø3Ø	STO5	35 Ø5	Ø58	X=Ø?	16-43
ØØ3	PRTX	-14	Ø31	STO6	35 Ø6	Ø59	GSBa	23 16 11
ØØ4	*LBLa	21 16 11	Ø32	STOA	35 11	Ø6Ø	GTOØ	22 ØØ
ØØ5	DSPØ	-63 ØØ	Ø33	STOC	35 13	Ø61	*LBLB	21 12
ØØ6	9	Ø9	Ø34	STOD	35 14	Ø62	1	Ø1
ØØ7	RCL4	36 Ø4	Ø35	*LBLØ	21 ØØ	Ø63	STOA	35 11
ØØ8	X>Y?	16-34	Ø36	RCL9	36 Ø9	Ø64	*LBLc	21 16 13
ØØ9	GTOb	22 16 12	Ø37	RCL6	36 Ø6	Ø65	RCLD	36 14
Ø1Ø	X<Ø?	16-45	Ø38	X=Y?	16-33	Ø66	X≠Ø?	16-42
Ø11	GTOb	22 16 12	Ø39	GTOc	22 16 13	Ø67	GTOc	22 16 13
Ø12	GSB3	23 Ø3	Ø4Ø	1	Ø1	Ø68	RCLC	36 13
Ø13	GSB9	23 Ø9	Ø41	ST+6	35-55 Ø6	Ø69	X≠Ø?	16-42
Ø14	PRTX	-14	Ø42	Ø	ØØ	Ø7Ø	GTOE	22 15
Ø15	RTN	24	Ø43	STOC	35 13	Ø71	*LBL6	21 Ø6
Ø16	*LBLb	21 16 12	Ø44	STOD	35 14	Ø72	RCL8	36 Ø8
Ø17	RCL4	36 Ø4	Ø45	*LBL7	21 Ø7	Ø73	RCL5	36 Ø5
Ø18	PRTX	-14	Ø46	Ø	ØØ	Ø74	X=Y?	16-33
Ø19	RCL5	36 Ø5	Ø47	STOA	35 11	Ø75	GTOd	22 16 14
Ø2Ø	PRTX	-14	Ø48	GSB1	23 Ø1	Ø76	RCLI	36 46
Ø21	RCL6	36 Ø6	Ø49	RCLE	36 15	Ø77	X≠Ø?	16-42
Ø22	PRTX	-14	Ø5Ø	X>Y?	16-34	Ø78	GTO2	22 Ø2
Ø23	RTN	24	Ø51	GTOB	22 12	Ø79	1	Ø1
Ø24	*LBLC	21 13	Ø52	X⇌Y	-41	Ø8Ø	STOC	35 13
Ø25	Ø	ØØ	Ø53	SPC	16-11	Ø81	ST+5	35-55 Ø5
Ø26	STO4	35 Ø4	Ø54	PRTX	-14	Ø82	Ø	ØØ
Ø27	STOI	35 46	Ø55	RCLI	36 46	Ø83	STO6	35 Ø6
Ø28	*LBL5	21 Ø5	Ø56	X≠Ø?	16-42	Ø84	GTO7	22 Ø7

Card 1. Monoclinic (Concluded)

Ø85	*LBLc	21 16 13	132	DSP4	-63 Ø4	178	CHS	-22
Ø86	RCLI	36 46	133	RCL4	36 Ø4	179	PRTX	-14
Ø87	X≠Ø?	16-42	134	RCLB	36 12	18Ø	RTN	24
Ø88	GTO4	22 Ø4	135	SIN	41	181	*LBL3	21 Ø3
Ø89	RCLA	36 11	136	STOØ	35 ØØ	182	9	Ø9
Ø9Ø	X=Ø?	16-43	137	÷	-24	183	RCL5	36 Ø5
Ø91	GTO6	22 Ø6	138	RCL1	36 Ø1	184	X>Y?	16-34
Ø92	GTOe	22 16 15	139	÷	-24	185	GTOb	22 16 12
Ø93	*LBLE	21 15	14Ø	X^2	53	186	X<Ø?	16-45
Ø94	RCLA	36 11	141	RCL5	36 Ø5	187	GTOb	22 16 12
Ø95	X=Ø?	16-43	142	RCL2	36 Ø2	188	9	Ø9
Ø96	GTO6	22 Ø6	143	÷	-24	189	RCL6	36 Ø6
Ø97	*LBLd	21 16 14	144	X^2	53	19Ø	X>Y?	16-34
Ø98	RCL7	36 Ø7	145	+	-55	191	GTOb	22 16 12
Ø99	RCL4	36 Ø4	146	RCL6	36 Ø6	192	X<Ø?	16-45
1ØØ	ABS	16 31	147	RCLØ	36 ØØ	193	GTOb	22 16 12
1Ø1	X=Y?	16-33	148	÷	-24	194	RCL4	36 Ø4
1Ø2	GTOe	22 16 15	149	RCL3	36 Ø3	195	1	Ø1
1Ø3	Ø	ØØ	15Ø	÷	-24	196	Ø	ØØ
1Ø4	STO5	35 Ø5	151	X^2	53	197	Ø	ØØ
1Ø5	1	Ø1	152	+	-55	198	x	-35
1Ø6	STOD	35 14	153	RCL4	36 Ø4	199	RTN	24
1Ø7	RCLI	36 46	154	2	Ø2	2ØØ	*LBL9	21 Ø9
1Ø8	X≠Ø?	16-42	155	x	-35	2Ø1	+	-55
1Ø9	GTO8	22 Ø8	156	RCL6	36 Ø6	2Ø2	RCL5	36 Ø5
11Ø	1	Ø1	157	x	-35	2Ø3	1	Ø1
111	ST+4	35-55 Ø4	158	RCLB	36 12	2Ø4	Ø	ØØ
112	Ø	ØØ	159	COS	42	2Ø5	x	-35
113	STO6	35 Ø6	16Ø	x	-35	2Ø6	+	-55
114	GTO7	22 Ø7	161	RCL1	36 Ø1	2Ø7	RTN	24
115	*LBLe	21 16 15	162	÷	-24	2Ø8	*LBL2	21 Ø2
116	RCLI	36 46	163	RCL3	36 Ø3	2Ø9	1	Ø1
117	X≠Ø?	16-42	164	÷	-24	21Ø	STO6	35 Ø6
118	R/S	51	165	RCLØ	36 ØØ	211	STOC	35 13
119	1	Ø1	166	X^2	53	212	ST+5	35-55 Ø5
12Ø	STOI	35 46	167	÷	-24	213	GTO7	22 Ø7
121	RCL7	36 Ø7	168	-	-45	214	*LBL4	21 Ø4
122	X=Ø?	16-43	169	1/X	52	215	RCLA	36 11
123	R/S	51	17Ø	ABS	16 31	216	X≠Ø?	16-42
124	RCL9	36 Ø9	171	√X	54	217	R/S	51
125	X=Ø?	16-43	172	RTN	24	218	GTO6	22 Ø6
126	R/S	51	173	*LBLD	21 14	219	*LBL8	21 Ø8
127	1	Ø1	174	DSPØ	-63 ØØ	22Ø	1	Ø1
128	CHS	-22	175	GSB3	23 Ø3	221	STO6	35 Ø6
129	STO4	35 Ø4	176	CHS	-22	222	ST-4	35-45 Ø4
13Ø	GTO5	22 Ø5	177	GSB9	23 Ø9	223	GTO7	22 Ø7
131	*LBL1	21 Ø1						

Card 2. Monoclinic

ØØ1	*LBLD	21 14	Ø52	+	-55	1Ø3	GTOb	22 16 12
ØØ2	RCL4	36 Ø4	Ø53	RCL4	36 Ø4	1Ø4	X<Ø?	16-45
ØØ3	RCL7	36 Ø7	Ø54	RCL6	36 Ø6	1Ø5	GTOb	22 16 12
ØØ4	x	-35	Ø55	GSB6	23 Ø6	1Ø6	RCL4	36 Ø4
ØØ5	RCL1	36 Ø1	Ø56	STOA	35 11	1Ø7	1	Ø1
ØØ6	X^2	53	Ø57	RCL7	36 Ø7	1Ø8	Ø	ØØ
ØØ7	÷	-24	Ø58	RCL1	36 Ø1	1Ø9	Ø	ØØ
ØØ8	RCL5	36 Ø5	Ø59	÷	-24	11Ø	x	-35
ØØ9	RCL8	36 Ø8	Ø6Ø	X^2	53	111	+	-55
Ø1Ø	x	-35	Ø61	RCL8	36 Ø8	112	RCL5	36 Ø5
Ø11	RCL2	36 Ø2	Ø62	GSB5	23 Ø5	113	1	Ø1
Ø12	X^2	53	Ø63	RCL9	36 Ø9	114	Ø	ØØ
Ø13	÷	-24	Ø64	RCL3	36 Ø3	115	x	-35
Ø14	RCLB	36 12	Ø65	÷	-24	116	+	-55
Ø15	SIN	41	Ø66	X^2	53	117	PRTX	-14
Ø16	X^2	53	Ø67	+	-55	118	GTOc	22 16 13
Ø17	x	-35	Ø68	RCL7	36 Ø7	119	*LBLb	21 16 12
Ø18	+	-55	Ø69	RCL9	36 Ø9	12Ø	RCL4	36 Ø4
Ø19	RCL6	36 Ø6	Ø7Ø	GSB6	23 Ø6	121	PRTX	-14
Ø2Ø	RCL9	36 Ø9	Ø71	RCLA	36 11	122	RCL5	36 Ø5
Ø21	x	-35	Ø72	x	-35	123	PRTX	-14
Ø22	RCL3	36 Ø3	Ø73	ABS	16 31	124	RCL6	36 Ø6
Ø23	X^2	53	Ø74	$\sqrt{X}$	54	125	PRTX	-14
Ø24	÷	-24	Ø75	RCLØ	36 ØØ	126	*LBLc	21 16 13
Ø25	+	-55	Ø76	X⇌Y	-41	127	9	Ø9
Ø26	RCL6	36 Ø6	Ø77	÷	-24	128	RCL7	36 Ø7
Ø27	RCL7	36 Ø7	Ø78	COS^{-1}	16 42	129	X>Y?	16-34
Ø28	x	-35	Ø79	9	Ø9	13Ø	GTOd	22 16 14
Ø29	RCL9	36 Ø9	Ø8Ø	Ø	ØØ	131	X<Ø?	16-45
Ø3Ø	RCL4	36 Ø4	Ø81	X⇌Y	-41	132	GTOd	22 16 14
Ø31	x	-35	Ø82	X>Y?	16-34	133	9	Ø9
Ø32	+	-55	Ø83	GSB1	23 Ø1	134	RCL8	36 Ø8
Ø33	RCLB	36 12	Ø84	SPC	16-11	135	X>Y?	16-34
Ø34	COS	42	Ø85	DSP2	-63 Ø2	136	GTOd	22 16 14
Ø35	x	-35	Ø86	PRTX	-14	137	X<Ø?	16-45
Ø36	RCL1	36 Ø1	Ø87	DSPØ	-63 ØØ	138	GTOd	22 16 14
Ø37	RCL3	36 Ø3	Ø88	9	Ø9	139	9	Ø9
Ø38	x	-35	Ø89	RCL4	36 Ø4	14Ø	RCL9	36 Ø9
Ø39	÷	-24	Ø9Ø	X>Y?	16-34	141	X>Y?	16-34
Ø4Ø	-	-45	Ø91	GTOb	22 16 12	142	GTOd	22 16 14
Ø41	STOØ	35 ØØ	Ø92	X<Ø?	16-45	143	X<Ø?	16-45
Ø42	RCL4	36 Ø4	Ø93	GTOb	22 16 12	144	GTOd	22 16 14
Ø43	RCL1	36 Ø1	Ø94	9	Ø9	145	RCL7	36 Ø7
Ø44	÷	-24	Ø95	RCL5	36 Ø5	146	1	Ø1
Ø45	X^2	53	Ø96	X>Y?	16-34	147	Ø	ØØ
Ø46	RCL5	36 Ø5	Ø97	GTOb	22 16 12	148	Ø	ØØ
Ø47	GSB5	23 Ø5	Ø98	X<Ø?	16-45	149	x	-35
Ø48	RCL6	36 Ø6	Ø99	GTOb	22 16 12	15Ø	+	-55
Ø49	RCL3	36 Ø3	1ØØ	9	Ø9	151	RCL8	36 Ø8
Ø5Ø	÷	-24	1Ø1	RCL6	36 Ø6	152	1	Ø1
Ø51	X^2	53	1Ø2	X>Y?	16-34	153	Ø	ØØ

Card 2. Monoclinic (Concluded)

154	x	-35	168	÷	-24	182	÷	-24
155	+	-55	169	RCLB	36 12	183	RCLB	36 12
156	PRTX	-14	17Ø	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 Ø7	173	+	-55	187	RTN	24
16Ø	PRTX	-14	174	RTN	24	188	*LBL1	21 Ø1
161	RCL8	36 Ø8	175	*LBL6	21 Ø6	189	1	Ø1
162	PRTX	-14	176	x	-35	19Ø	8	Ø8
163	RCL9	36 Ø9	177	2	Ø2	191	Ø	ØØ
164	PRTX	-14	178	x	-35	192	X⇌Y	-41
165	RTN	24	179	RCL1	36 Ø1	193	-	-45
166	*LBL5	21 Ø5	18Ø	÷	-24	194	RTN	24
167	RCL2	36 Ø2	181	RCL3	36 Ø3	195	R/S	51

Card 3. Monoclinic

ØØ1	*LBLE	21 15	Ø36	+	-55	Ø71	x	-35
ØØ2	RCL4	36 Ø4	Ø37	STOØ	35 ØØ	Ø72	+	-55
ØØ3	RCL7	36 Ø7	Ø38	RCL4	36 Ø4	Ø73	RCLA	36 11
ØØ4	x	-35	Ø39	RCL1	36 Ø1	Ø74	x	-35
ØØ5	RCL1	36 Ø1	Ø4Ø	x	-35	Ø75	ABS	16 31
ØØ6	X^2	53	Ø41	X^2	53	Ø76	$\sqrt{X}$	54
ØØ7	x	-35	Ø42	RCL5	36 Ø5	Ø77	RCLØ	36 ØØ
ØØ8	RCL5	36 Ø5	Ø43	RCL2	36 Ø2	Ø78	X⇌Y	-41
ØØ9	RCL8	36 Ø8	Ø44	x	-35	Ø79	÷	-24
Ø1Ø	x	-35	Ø45	X^2	53	Ø8Ø	COS^{-1}	16 42
Ø11	RCL2	36 Ø2	Ø46	+	-55	Ø81	9	Ø9
Ø12	X^2	53	Ø47	RCL6	36 Ø6	Ø82	Ø	ØØ
Ø13	x	-35	Ø48	RCL3	36 Ø3	Ø83	X⇌Y	-41
Ø14	+	-55	Ø49	GSB7	23 Ø7	Ø84	X>Y?	16-34
Ø15	RCL6	36 Ø6	Ø5Ø	RCL4	36 Ø4	Ø85	GSB1	23 Ø1
Ø16	RCL9	36 Ø9	Ø51	x	-35	Ø86	SPC	16-11
Ø17	x	-35	Ø52	RCL6	36 Ø6	Ø87	DSP2	-63 Ø2
Ø18	RCL3	36 Ø3	Ø53	x	-35	Ø88	PRTX	-14
Ø19	X^2	53	Ø54	+	-55	Ø89	DSPØ	-63 ØØ
Ø2Ø	x	-35	Ø55	STOA	35 11	Ø9Ø	9	Ø9
Ø21	+	-55	Ø56	RCL7	36 Ø7	Ø91	RCL4	36 Ø4
Ø22	RCL6	36 Ø6	Ø57	RCL1	36 Ø1	Ø92	X>Y?	16-34
Ø23	RCL7	36 Ø7	Ø58	x	-35	Ø93	GTOb	22 16 12
Ø24	x	-35	Ø59	X^2	53	Ø94	X<Ø?	16-45
Ø25	RCL9	36 Ø9	Ø6Ø	RCL8	36 Ø8	Ø95	GTOb	22 16 12
Ø26	RCL4	36 Ø4	Ø61	RCL2	36 Ø2	Ø96	9	Ø9
Ø27	x	-35	Ø62	x	-35	Ø97	RCL5	36 Ø5
Ø28	+	-55	Ø63	X^2	53	Ø98	X>Y?	16-34
Ø29	RCLB	36 12	Ø64	+	-55	Ø99	GTOb	22 16 12
Ø3Ø	COS	42	Ø65	RCL9	36 Ø9	1ØØ	X<Ø?	16-45
Ø31	x	-35	Ø66	RCL3	36 Ø3	1Ø1	GTOb	22 16 12
Ø32	RCL1	36 Ø1	Ø67	GSB7	23 Ø7	1Ø2	9	Ø9
Ø33	RCL3	36 Ø3	Ø68	RCL7	36 Ø7	1Ø3	RCL6	36 Ø6
Ø34	x	-35	Ø69	x	-35	1Ø4	X>Y?	16-34
Ø35	x	-35	Ø7Ø	RCL9	36 Ø9	1Ø5	GTOb	22 16 12

Card 3. Monoclinic (Concluded)

1Ø6	X<Ø?	16-45	134	GTOd	22 16 14	162	PRTX	-14
1Ø7	GTOb	22 16 12	135	9	Ø9	163	RCL8	36 Ø8
1Ø8	RCL4	36 Ø4	136	RCL8	36 Ø8	164	PRTX	-14
1Ø9	1	Ø1	137	X>Y?	16-34	165	RCL9	36 Ø9
11Ø	Ø	ØØ	138	GTOd	22 16 14	166	PRTX	-14
111	Ø	ØØ	139	X<Ø?	16-45	167	RTN	24
112	x	-35	14Ø	GTOd	22 16 14	168	*LBL7	21 Ø7
113	+	-55	141	9	Ø9	169	x	-35
114	RCL5	36 Ø5	142	RCL9	36 Ø9	17Ø	X^2	53
115	1	Ø1	143	X>Y?	16-34	171	+	-55
116	Ø	ØØ	144	GTOd	22 16 14	172	RCL1	36 Ø1
117	x	-35	145	X<Ø?	16-45	173	2	Ø2
118	+	-55	146	GTOd	22 16 14	174	x	-35
119	PRTX	-14	147	RCL7	36 Ø7	175	RCL3	36 Ø3
12Ø	GTOc	22 16 13	148	1	Ø1	176	x	-35
121	*LBLb	21 16 12	149	Ø	ØØ	177	RCLB	36 12
122	RCL4	36 Ø4	15Ø	Ø	ØØ	178	COS	42
123	PRTX	-14	151	x	-35	179	x	-35
124	RCL5	36 Ø5	152	+	-55	18Ø	RTN	24
125	PRTX	-14	153	RCL8	36 Ø8	181	*LBL1	21 Ø1
126	RCL6	36 Ø6	154	1	Ø1	182	1	Ø1
127	PRTX	-14	155	Ø	ØØ	183	8	Ø8
128	*LBLc	21 16 13	156	x	-35	184	Ø	ØØ
129	9	Ø9	157	+	-55	185	X⇌Y	-41
13Ø	RCL7	36 Ø7	158	PRTX	-14	186	-	-45
131	X>Y?	16-34	159	RTN	24	187	RTN	24
132	GTOd	22 16 14	16Ø	*LBLd	21 16 14	188	R/S	51
133	X<Ø?	16-45	161	RCL7	36 Ø7			

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:

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

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

$$A_{hkl} = [h^2b^2c^2\sin^2\alpha + k^2a^2c^2\sin^2\beta + l^2a^2b^2\sin^2\gamma$$
$$+ 2hkabc^2(\cos\alpha\cos\beta - \cos\gamma)$$
$$+ 2hlab^2c(\cos\gamma\cos\alpha - \cos\beta)$$
$$+ 2kla^2bc(\cos\beta\cos\gamma - \cos\alpha)]^{1/2}$$

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

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 Card 1 Calculate d	Register 1- a Register 2- b Register 3- c Register 4- h Register 5- k Register 6- l Register A- α Register B- β Register C- γ	d h k l
Label C Card 1 Calculate all possible d's within limits	Register 1- a Register 2- b 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 A- α Register B- β Register C- γ Register E- only d values larger than this printed	d h k l
Label D[a] Card 2 Calculate angle (ϕ) between crystal planes	Register 1- a Register 2- b Register 3- c Register 4- h_1 Register 5- k_1 Register 6- l_1 Register 7- h_2 Register 8- k_2 Register 9- l_2 Register A- α Register B- β Register C- γ	ϕ or ϕ $h_1k_1l_1$ h_1 h_2 k_1 k_2 l_1 l_2 h_2 k_2 l_2
Label E[a] Card 3 Calculate angle (ρ) between crystal zones	Register 1- a Register 2- b Register 3- c Register 4- u_1 Register 5- v_1 Register 6- w_1 Register 7- u_2 Register 8- v_2 Register 9- w_2 Register A- α	ρ or ρ $u_1v_1w_1$ u_1 $u_2v_2w_2$ v_1 w_1 u_2 v_2 w_2

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

[a] If h, k, and 1 (u, v, and w) are zero or positive and less than 10, output is in the form hkl (uvw). If h, k, or 1 (u, v, or w) are negative, or greater than 9, output is in the form $\begin{matrix} h & u \\ k \text{ or } & v \\ 1 & w \end{matrix}$.

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

ØØ1	*LBLA	21 11	Ø36	RCL5	36 Ø5	Ø71	CHS	-22
ØØ2	GSBe	23 16 15	Ø37	+	-55	Ø72	STO5	35 Ø5
ØØ3	*LBLc	21 16 13	Ø38	X=Ø?	16-43	Ø73	RCL6	36 Ø6
ØØ4	SPC	16-11	Ø39	GTO5	22 Ø5	Ø74	X=Ø?	16-43
ØØ5	DSP4	-63 Ø4	Ø4Ø	RCL6	36 Ø6	Ø75	GTO5	22 Ø5
ØØ6	PRTX	-14	Ø41	CHS	-22	Ø76	RCL4	36 Ø4
ØØ7	DSPØ	-63 ØØ	Ø42	STO6	35 Ø6	Ø77	CHS	-22
ØØ8	RCL4	36 Ø4	Ø43	X=Ø?	16-43	Ø78	STO4	35 Ø4
ØØ9	PRTX	-14	Ø44	GTOd	22 16 14	Ø79	GSBe	23 16 15
Ø1Ø	RCL5	36 Ø5	Ø45	GSBe	23 16 15	Ø8Ø	RCLE	36 15
Ø11	PRTX	-14	Ø46	RCLE	36 15	Ø81	X>Y?	16-34
Ø12	RCL6	36 Ø6	Ø47	X>Y?	16-34	Ø82	GTOE	22 15
Ø13	PRTX	-14	Ø48	GTOd	22 16 14	Ø83	X⇌Y	-41
Ø14	RTN	24	Ø49	X⇌Y	-41	Ø84	GSBc	23 16 13
Ø15	*LBLC	21 13	Ø5Ø	GSBc	23 16 13	Ø85	*LBLE	21 15
Ø16	Ø	ØØ	Ø51	*LBLd	21 16 14	Ø86	RCL4	36 Ø4
Ø17	STO4	35 Ø4	Ø52	RCL6	36 Ø6	Ø87	CHS	-22
Ø18	STO5	35 Ø5	Ø53	CHS	-22	Ø88	STO4	35 Ø4
Ø19	STO6	35 Ø6	Ø54	STO6	35 Ø6	Ø89	GTO5	22 Ø5
Ø2Ø	*LBL5	21 Ø5	Ø55	RCL4	36 Ø4	Ø9Ø	*LBL9	21 Ø9
Ø21	RCL9	36 Ø9	Ø56	X=Ø?	16-43	Ø91	RCL8	36 Ø8
Ø22	RCL6	36 Ø6	Ø57	GTO5	22 Ø5	Ø92	RCL5	36 Ø5
Ø23	X=Y?	16-33	Ø58	RCL5	36 Ø5	Ø93	X=Y?	16-33
Ø24	GTO9	22 Ø9	Ø59	X=Ø?	16-43	Ø94	GTO8	22 Ø8
Ø25	1	Ø1	Ø6Ø	GTO5	22 Ø5	Ø95	1	Ø1
Ø26	ST+6	35-55 Ø6	Ø61	CHS	-22	Ø96	ST+5	35-55 Ø5
Ø27	*LBL6	21 Ø6	Ø62	STO5	35 Ø5	Ø97	Ø	ØØ
Ø28	GSBe	23 16 15	Ø63	GSBe	23 16 13	Ø98	STO6	35 Ø6
Ø29	RCLE	36 15	Ø64	RCLE	36 15	Ø99	GTO6	22 Ø6
Ø3Ø	X>Y?	16-34	Ø65	X>Y?	16-34	1ØØ	*LBL8	21 Ø8
Ø31	GTO4	22 Ø4	Ø66	GTO3	22 Ø3	1Ø1	RCL7	36 Ø7
Ø32	X⇌Y	-41	Ø67	X⇌Y	-41	1Ø2	RCL4	36 Ø4
Ø33	GSBc	23 16 13	Ø68	GSBc	23 16 13	1Ø3	X=Y?	16-33
Ø34	*LBL4	21 Ø4	Ø69	*LBL3	21 Ø3	1Ø4	R/S	51
Ø35	RCL4	36 Ø4	Ø7Ø	RCL5	36 Ø5	1Ø5	1	Ø1

Card 1. Triclinic (Concluded)

1Ø6	ST+4	35-55 Ø4	143	RCL1	36 Ø1	18Ø	RCL6	36 Ø6
1Ø7	Ø	ØØ	144	RCL2	36 Ø2	181	GSB2	23 Ø2
1Ø8	STO5	35 Ø5	145	x	-35	182	RCLI	36 46
1Ø9	STO6	35 Ø6	146	RCLC	36 13	183	RCLØ	36 ØØ
11Ø	GTO6	22 Ø6	147	SIN	41	184	x	-35
111	*LBL1	21 Ø1	148	x	-35	185	RCLD	36 14
112	RCL1	36 Ø1	149	RCL6	36 Ø6	186	-	-45
113	x	-35	15Ø	x	-35	187	GSB1	23 Ø1
114	*LBLb	21 16 12	151	X^2	53	188	RCL2	36 Ø2
115	RCL2	36 Ø2	152	+	-55	189	x	-35
116	x	-35	153	RCLA	36 11	19Ø	RCL6	36 Ø6
117	*LBLa	21 16 11	154	COS	42	191	x	-35
118	RCL3	36 Ø3	155	STOØ	35 ØØ	192	RCL4	36 Ø4
119	x	-35	156	RCLB	36 12	193	GSB2	23 Ø2
12Ø	RTN	24	157	COS	42	194	RCLØ	36 ØØ
121	*LBL2	21 Ø2	158	STOD	35 14	195	X^2	53
122	x	-35	159	x	-35	196	CHS	-22
123	2	Ø2	16Ø	RCLC	36 13	197	1	Ø1
124	x	-35	161	COS	42	198	+	-55
125	+	-55	162	STOI	35 46	199	RCLD	36 14
126	RTN	24	163	-	-45	2ØØ	X^2	53
127	*LBLe	21 16 15	164	GSB1	23 Ø1	2Ø1	-	-45
128	RCLA	36 11	165	GSBa	23 16 11	2Ø2	RCLI	36 46
129	SIN	41	166	RCL4	36 Ø4	2Ø3	X^2	53
13Ø	GSBb	23 16 12	167	x	-35	2Ø4	-	-45
131	RCL4	36 Ø4	168	RCL5	36 Ø5	2Ø5	RCLØ	36 ØØ
132	x	-35	169	GSB2	23 Ø2	2Ø6	RCLD	36 14
133	X^2	53	17Ø	RCLD	36 14	2Ø7	x	-35
134	RCL1	36 Ø1	171	RCLI	36 46	2Ø8	RCLI	36 46
135	GSBa	23 16 11	172	x	-35	2Ø9	GSB2	23 Ø2
136	RCLB	36 12	173	RCLØ	36 ØØ	21Ø	GSB1	23 Ø1
137	SIN	41	174	-	-45	211	GSB1	23 Ø1
138	x	-35	175	GSB1	23 Ø1	212	X⇌Y	-41
139	RCL5	36 Ø5	176	RCL1	36 Ø1	213	÷	-24
14Ø	x	-35	177	x	-35	214	ABS	16 31
141	X^2	53	178	RCL5	36 Ø5	215	√X	54
142	+	-55	179	x	-35	216	RTN	24

Card 2. Triclinic

ØØ1	*LBLD	21 14	Ø13	GSBe	23 16 15	Ø25	RCL8	36 Ø8
ØØ2	RCL4	36 Ø4	Ø14	RCL5	36 Ø5	Ø26	GSBd	23 16 14
ØØ3	GSBa	23 16 11	Ø15	RCL6	36 Ø6	Ø27	RCL7	36 Ø7
ØØ4	RCL5	36 Ø5	Ø16	GSBE	23 15	Ø28	RCL9	36 Ø9
ØØ5	GSBb	23 16 12	Ø17	STOI	35 46	Ø29	GSBe	23 16 15
ØØ6	RCL6	36 Ø6	Ø18	RCL7	36 Ø7	Ø3Ø	RCL8	36 Ø8
ØØ7	GSBc	23 16 13	Ø19	GSBa	23 16 11	Ø31	RCL9	36 Ø9
ØØ8	RCL4	36 Ø4	Ø2Ø	RCL8	36 Ø8	Ø32	GSBE	23 15
ØØ9	RCL5	36 Ø5	Ø21	GSBb	23 16 12	Ø33	RCLI	36 46
Ø1Ø	GSBd	23 16 14	Ø22	RCL9	36 Ø9	Ø34	x	-35
Ø11	RCL4	36 Ø4	Ø23	GSBc	23 16 13	Ø35	ABS	16 31
Ø12	RCL6	36 Ø6	Ø24	RCL7	36 Ø7	Ø36	√X	54

Card 2. Triclinic (Continued)

Ø37	STOI	35 46	Ø88	GSB4	23 Ø4	139	GSBA	23 11
Ø38	RCL2	36 Ø2	Ø89	RCLI	36 46	14Ø	RTN	24
Ø39	GSBA	23 11	Ø9Ø	÷	-24	141	*LBLa	21 16 11
Ø4Ø	RCLA	36 11	Ø91	COS^{-1}	16 42	142	GSBB	23 12
Ø41	SIN	41	Ø92	PRTX	-14	143	GSBA	23 11
Ø42	GSB6	23 Ø6	Ø93	RCL4	36 Ø4	144	RCLA	36 11
Ø43	RCL4	36 Ø4	Ø94	X<Ø?	16-45	145	SIN	41
Ø44	x	-35	Ø95	GTO8	22 Ø8	146	GSB6	23 Ø6
Ø45	RCL7	36 Ø7	Ø96	9	Ø9	147	RTN	24
Ø46	x	-35	Ø97	RCL5	36 Ø5	148	*LBLb	21 16 12
Ø47	RCL1	36 Ø1	Ø98	X>Y?	16-34	149	RCL1	36 Ø1
Ø48	GSBA	23 11	Ø99	GTO8	22 Ø8	15Ø	x	-35
Ø49	RCLB	36 12	1ØØ	X<Ø?	16-45	151	GSBA	23 11
Ø5Ø	SIN	41	1Ø1	GTO8	22 Ø8	152	RCLB	36 12
Ø51	GSB6	23 Ø6	1Ø2	9	Ø9	153	SIN	41
Ø52	RCL5	36 Ø5	1Ø3	RCL6	36 Ø6	154	GSB6	23 Ø6
Ø53	x	-35	1Ø4	X>Y?	16-34	155	+	-55
Ø54	RCL8	36 Ø8	1Ø5	GTO8	22 Ø8	156	RTN	24
Ø55	GSB7	23 Ø7	1Ø6	X<Ø?	16-45	157	*LBLc	21 16 13
Ø56	RCL1	36 Ø1	1Ø7	GTO8	22 Ø8	158	RCL1	36 Ø1
Ø57	GSBB	23 12	1Ø8	RCL4	36 Ø4	159	x	-35
Ø58	RCLC	36 13	1Ø9	1	Ø1	16Ø	GSBB	23 12
Ø59	SIN	41	11Ø	Ø	ØØ	161	RCLC	36 13
Ø6Ø	GSB6	23 Ø6	111	Ø	ØØ	162	SIN	41
Ø61	RCL6	36 Ø6	112	GSB7	23 Ø7	163	GSB6	23 Ø6
Ø62	x	-35	113	RCL5	36 Ø5	164	+	-55
Ø63	RCL9	36 Ø9	114	1	Ø1	165	RTN	24
Ø64	GSB7	23 Ø7	115	Ø	ØØ	166	*LBLd	21 16 14
Ø65	RCL5	36 Ø5	116	GSB7	23 Ø7	167	x	-35
Ø66	RCL7	36 Ø7	117	PRTX	-14	168	GSBA	23 11
Ø67	x	-35	118	*LBL9	21 Ø9	169	2	Ø2
Ø68	RCL4	36 Ø4	119	RCL7	36 Ø7	17Ø	*LBL2	21 Ø2
Ø69	RCL8	36 Ø8	12Ø	PRTX	-14	171	GSB1	23 Ø1
Ø7Ø	GSB7	23 Ø7	121	RCL8	36 Ø8	172	RCLA	36 11
Ø71	RCL3	36 Ø3	122	PRTX	-14	173	COS	42
Ø72	GSB2	23 Ø2	123	RCL9	36 Ø9	174	STOD	35 14
Ø73	RCL4	36 Ø4	124	PRTX	-14	175	RCLB	36 12
Ø74	RCL9	36 Ø9	125	RTN	24	176	COS	42
Ø75	x	-35	126	*LBL8	21 Ø8	177	STOE	35 15
Ø76	RCL6	36 Ø6	127	RCL4	36 Ø4	178	x	-35
Ø77	RCL7	36 Ø7	128	PRTX	-14	179	RCLC	36 13
Ø78	GSB7	23 Ø7	129	RCL5	36 Ø5	18Ø	COS	42
Ø79	RCL2	36 Ø2	13Ø	PRTX	-14	181	STOØ	35 ØØ
Ø8Ø	GSB3	23 Ø3	131	RCL6	36 Ø6	182	GTO5	22 Ø5
Ø81	RCL5	36 Ø5	132	PRTX	-14	183	*LBLe	21 16 15
Ø82	RCL9	36 Ø9	133	GTO9	22 Ø9	184	x	-35
Ø83	x	-35	134	*LBL1	21 Ø1	185	GSBB	23 12
Ø84	RCL6	36 Ø6	135	x	-35	186	2	Ø2
Ø85	RCL8	36 Ø8	136	RCL1	36 Ø1	187	*LBL3	21 Ø3
Ø86	GSB7	23 Ø7	137	x	-35	188	GSB1	23 Ø1
Ø87	RCL1	36 Ø1	138	GSBB	23 12	189	RCLØ	36 ØØ

Card 2. Triclinic (Concluded)

19Ø	RCLD	36 14	2Ø2	RCLØ	36 ØØ	214	x	-35
191	x	-35	2Ø3	x	-35	215	+	-55
192	RCLE	36 15	2Ø4	RCLD	36 14	216	RTN	24
193	GTO5	22 Ø5	2Ø5	*LBL5	21 Ø5	217	*LBLA	21 11
194	*LBLE	21 15	2Ø6	-	-45	218	RCL3	36 Ø3
195	x	-35	2Ø7	GSB7	23 Ø7	219	x	-35
196	RCL1	36 Ø1	2Ø8	RTN	24	22Ø	RTN	24
197	x	-35	2Ø9	*LBL6	21 Ø6	221	*LBLB	21 12
198	2	Ø2	21Ø	x	-35	222	RCL2	36 Ø2
199	*LBL4	21 Ø4	211	X^2	53	223	x	-35
2ØØ	GSB1	23 Ø1	212	RTN	24	224	RTN	24
2Ø1	RCLE	36 15	213	*LBL7	21 Ø7			

Card 3. Triclinic

ØØ1	*LBLE	21 15	Ø38	RCL7	36 Ø7	Ø75	RCL9	36 Ø9
ØØ2	RCL4	36 Ø4	Ø39	GSBb	23 16 12	Ø76	RCL3	36 Ø3
ØØ3	RCL7	36 Ø7	Ø4Ø	GSB3	23 Ø3	Ø77	GSBa	23 16 11
ØØ4	x	-35	Ø41	STOØ	35 ØØ	Ø78	RCL8	36 Ø8
ØØ5	RCL1	36 Ø1	Ø42	RCL4	36 Ø4	Ø79	GSBc	23 16 13
ØØ6	X^2	53	Ø43	RCL1	36 Ø1	Ø8Ø	RCL9	36 Ø9
ØØ7	x	-35	Ø44	x	-35	Ø81	x	-35
ØØ8	RCL5	36 Ø5	Ø45	X^2	53	Ø82	GSB1	23 Ø1
ØØ9	RCL8	36 Ø8	Ø46	RCL5	36 Ø5	Ø83	RCL7	36 Ø7
Ø1Ø	x	-35	Ø47	RCL2	36 Ø2	Ø84	GSBc	23 16 13
Ø11	RCL2	36 Ø2	Ø48	GSBa	23 16 11	Ø85	RCL9	36 Ø9
Ø12	X^2	53	Ø49	RCL6	36 Ø6	Ø86	x	-35
Ø13	GSBb	23 16 12	Ø5Ø	RCL3	36 Ø3	Ø87	GSB2	23 Ø2
Ø14	RCL6	36 Ø6	Ø51	GSBa	23 16 11	Ø88	RCL7	36 Ø7
Ø15	RCL9	36 Ø9	Ø52	RCL5	36 Ø5	Ø89	GSBc	23 16 13
Ø16	x	-35	Ø53	GSBc	23 16 13	Ø9Ø	RCL8	36 Ø8
Ø17	RCL3	36 Ø3	Ø54	RCL6	36 Ø6	Ø91	x	-35
Ø18	X^2	53	Ø55	x	-35	Ø92	GSB3	23 Ø3
Ø19	GSBb	23 16 12	Ø56	GSB1	23 Ø1	Ø93	RCLI	36 46
Ø2Ø	RCL5	36 Ø5	Ø57	RCL4	36 Ø4	Ø94	x	-35
Ø21	RCL9	36 Ø9	Ø58	GSBc	23 16 13	Ø95	ABS	16 31
Ø22	x	-35	Ø59	RCL6	36 Ø6	Ø96	$\sqrt{X}$	54
Ø23	RCL6	36 Ø6	Ø6Ø	x	-35	Ø97	RCLØ	36 ØØ
Ø24	RCL8	36 Ø8	Ø61	GSB2	23 Ø2	Ø98	X⇌Y	-41
Ø25	GSBb	23 16 12	Ø62	RCL4	36 Ø4	Ø99	÷	-24
Ø26	GSB1	23 Ø1	Ø63	GSBc	23 16 13	1ØØ	COS^{-1}	16 42
Ø27	RCL6	36 Ø6	Ø64	RCL5	36 Ø5	1Ø1	SPC	16-11
Ø28	RCL7	36 Ø7	Ø65	x	-35	1Ø2	DSP2	-63 Ø2
Ø29	x	-35	Ø66	GSB3	23 Ø3	1Ø3	PRTX	-14
Ø3Ø	RCL4	36 Ø4	Ø67	STOI	35 46	1Ø4	DSPØ	-63 ØØ
Ø31	RCL9	36 Ø9	Ø68	RCL7	36 Ø7	1Ø5	9	Ø9
Ø32	GSBb	23 16 12	Ø69	RCL1	36 Ø1	1Ø6	RCL4	36 Ø4
Ø33	GSB2	23 Ø2	Ø7Ø	x	-35	1Ø7	X>Y?	16-34
Ø34	RCL4	36 Ø4	Ø71	X^2	53	1Ø8	GTO7	22 Ø7
Ø35	RCL8	36 Ø8	Ø72	RCL8	36 Ø8	1Ø9	X<Ø?	16-45
Ø36	x	-35	Ø73	RCL2	36 Ø2	11Ø	GTO7	22 Ø7
Ø37	RCL5	36 Ø5	Ø74	GSBa	23 16 11	111	9	Ø9

Card 3. Triclinic (Concluded)

112	RCL5	36 Ø5	15Ø	9	Ø9	187	RCL2	36 Ø2
113	X>Y?	16-34	151	RCL8	36 Ø8	188	x	-35
114	GTO7	22 Ø7	152	X>Y?	16-34	189	RCL3	36 Ø3
115	X<Ø?	16-45	153	GTO9	22 Ø9	19Ø	GSBb	23 16 12
116	GTO7	22 Ø7	154	X<Ø?	16-45	191	RTN	24
117	9	Ø9	155	GTO9	22 Ø9	192	*LBL2	21 Ø2
118	RCL6	36 Ø6	156	9	Ø9	193	RCLB	36 12
119	X>Y?	16-34	157	RCL9	36 Ø9	194	COS	42
12Ø	GTO7	22 Ø7	158	X>Y?	16-34	195	x	-35
121	X<Ø?	16-45	159	GTO9	22 Ø9	196	RCL1	36 Ø1
122	GTO7	22 Ø7	16Ø	X<Ø?	16-45	197	x	-35
123	RCL4	36 Ø4	161	GTO9	22 Ø9	198	RCL3	36 Ø3
124	1	Ø1	162	RCL7	36 Ø7	199	GSBb	23 16 12
125	Ø	ØØ	163	1	Ø1	2ØØ	RTN	24
126	Ø	ØØ	164	Ø	ØØ	2Ø1	*LBL3	21 Ø3
127	x	-35	165	Ø	ØØ	2Ø2	RCLC	36 13
128	+	-55	166	x	-35	2Ø3	COS	42
129	RCL5	36 Ø5	167	+	-55	2Ø4	x	-35
13Ø	1	Ø1	168	RCL8	36 Ø8	2Ø5	RCL1	36 Ø1
131	0	ØØ	169	1	Ø1	2Ø6	x	-35
132	x	-35	170	Ø	ØØ	2Ø7	RCL2	36 Ø2
133	+	-55	171	x	-35	2Ø8	GSBb	23 16 12
134	PRTX	-14	172	+	-55	2Ø9	RTN	24
135	GTO8	22 Ø8	173	PRTX	-14	21Ø	*LBLa	21 16 11
136	*LBL7	21 Ø7	174	RTN	24	211	x	-35
137	RCL4	36 Ø4	175	*LBL9	21 Ø9	212	X^2	53
138	PRTX	-14	176	RCL7	36 Ø7	213	+	-55
139	RCL5	36 Ø5	177	PRTX	-14	214	RTN	24
14Ø	PRTX	-14	178	RCL8	36 Ø8	215	*LBLb	21 16 12
141	RCL6	36 Ø6	179	PRTX	-14	216	x	-35
142	PRTX	-14	18Ø	RCL9	36 Ø9	217	+	-55
143	*LBL8	21 Ø8	181	PRTX	-14	218	RTN	24
144	9	Ø9	182	RTN	24	219	*LBLc	21 16 13
145	RCL7	36 Ø7	183	*LBL1	21 Ø1	22Ø	2	Ø2
146	X>Y?	16-34	184	RCLA	36 11	221	x	-35
147	GTO9	22 Ø9	185	COS	42	222	RTN	24
148	X<Ø?	16-45	186	x	-35	223	R/S	51
149	GTO9	22 Ø9						

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		
TRICLINIC	Register 1- α	a
	Register 2- β	b
	Register 3- γ	c
	Register 4- a	α
	Register 5- b	β
	Register 6- c	γ
		$a'(\partial_{100})$
		$b'(\partial_{010})$
		$c'(\partial_{001})$
		α'
		β'
		γ'
Label B		
MONOCLINIC	Register 2- β	a
	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 RHOMBOHEDRAL	Register 1- α_{rh} Register 4- a_{hex} Register 5- a_{rh} Register 6- c_{hex}	a_{hex} c_{hex} a_{rh} α_{rh} $a'_{rh}(\partial_{001})$ α'_{rh}
Label D HEXAGONAL	Register 4- a Register 6- c	a 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

ØØ1	*LBLA	21 11	Ø26	RCL1	36 Ø1	Ø51	SIN	41
ØØ2	GSB1	23 Ø1	Ø27	COS	42	Ø52	÷	-24
ØØ3	RCL1	36 Ø1	Ø28	RCL3	36 Ø3	Ø53	RCL2	36 Ø2
ØØ4	GSB5	23 Ø5	Ø29	COS	42	Ø54	SIN	41
ØØ5	RCL2	36 Ø2	Ø3Ø	x	-35	Ø55	÷	-24
ØØ6	PRTX	-14	Ø31	RCL2	36 Ø2	Ø56	COS^{-1}	16 42
ØØ7	RCL3	36 Ø3	Ø32	COS	42	Ø57	STO9	35 Ø9
ØØ8	PRTX	-14	Ø33	-	-45	Ø58	1	Ø1
ØØ9	GSB7	23 Ø7	Ø34	RCL1	36 Ø1	Ø59	ENT↑	-21
Ø1Ø	RCL2	36 Ø2	Ø35	SIN	41	Ø6Ø	RCL1	36 Ø1
Ø11	COS	42	Ø36	÷	-24	Ø61	COS	42
Ø12	RCL3	36 Ø3	Ø37	RCL3	36 Ø3	Ø62	X^2	53
Ø13	COS	42	Ø38	SIN	41	Ø63	-	-45
Ø14	x	-35	Ø39	÷	-24	Ø64	RCL2	36 Ø2
Ø15	RCL1	36 Ø1	Ø4Ø	COS^{-1}	16 42	Ø65	COS	42
Ø16	COS	42	Ø41	STO8	35 Ø8	Ø66	X^2	53
Ø17	-	-45	Ø42	RCL1	36 Ø1	Ø67	-	-45
Ø18	RCL2	36 Ø2	Ø43	COS	42	Ø68	RCL3	36 Ø3
Ø19	SIN	41	Ø44	RCL2	36 Ø2	Ø69	COS	42
Ø2Ø	÷	-24	Ø45	COS	42	Ø7Ø	X^2	53
Ø21	RCL3	36 Ø3	Ø46	x	-35	Ø71	-	-45
Ø22	SIN	41	Ø47	RCL3	36 Ø3	Ø72	RCL1	36 Ø1
Ø23	÷	-24	Ø48	COS	42	Ø73	COS	42
Ø24	COS^{-1}	16 42	Ø49	-	-45	Ø74	2	Ø2
Ø25	STO7	35 Ø7	Ø5Ø	RCL1	36 Ø1	Ø75	x	-35

Apparent Crystal Parameters (Continued)

Ø76	RCL2	36 Ø2	123	*LBLC	21 13	17Ø	PRTX	-14
Ø77	COS	42	124	GSB6	23 Ø6	171	SPC	16-11
Ø78	x	-35	125	RCL4	36 Ø4	172	3	Ø3
Ø79	RCL3	36 Ø3	126	GSB4	23 Ø4	173	ENT↑	-21
Ø8Ø	COS	42	127	RCL6	36 Ø6	174	4	Ø4
Ø81	x	-35	128	PRTX	-14	175	÷	-24
Ø82	+	-55	129	SPC	16-11	176	√X	54
Ø83	√X	54	13Ø	RCL5	36 Ø5	177	RCL4	36 Ø4
Ø84	STOØ	35 ØØ	131	PRTX	-14	178	x	-35
Ø85	RCL4	36 Ø4	132	RCL1	36 Ø1	179	PRTX	-14
Ø86	RCL1	36 Ø1	133	GSB5	23 Ø5	18Ø	RCL6	36 Ø6
Ø87	GSB2	23 Ø2	134	GSB7	23 Ø7	181	PRTX	-14
Ø88	RCL5	36 Ø5	135	GSB3	23 Ø3	182	RTN	24
Ø89	RCL2	36 Ø2	136	.	-62	183	*LBL1	21 Ø1
Ø9Ø	GSB2	23 Ø2	137	5	Ø5	184	GSB6	23 Ø6
Ø91	RCL6	36 Ø6	138	-	-45	185	RCL4	36 Ø4
Ø92	RCL3	36 Ø3	139	GSB3	23 Ø3	186	GSB4	23 Ø4
Ø93	GSB2	23 Ø2	14Ø	1	Ø1	187	RCL5	36 Ø5
Ø94	SPC	16-11	141	+	-55	188	PRTX	-14
Ø95	RCL7	36 Ø7	142	÷	-24	189	RCL6	36 Ø6
Ø96	GSB5	23 Ø5	143	COS^{-1}	16 42	19Ø	PRTX	-14
Ø97	RCL8	36 Ø8	144	STOI	35 46	191	SPC	16-11
Ø98	PRTX	-14	145	RCL1	36 Ø1	192	RTN	24
Ø99	RCL9	36 Ø9	146	COS	42	193	*LBL2	21 Ø2
1ØØ	PRTX	-14	147	X^2	53	194	SIN	41
1Ø1	RTN	24	148	2	Ø2	195	÷	-24
1Ø2	*LBLB	21 12	149	x	-35	196	RCLØ	36 ØØ
1Ø3	GSB1	23 Ø1	15Ø	RCL1	36 Ø1	197	x	-35
1Ø4	RCL2	36 Ø2	151	COS	42	198	GSB4	23 Ø4
1Ø5	GSB5	23 Ø5	152	1	Ø1	199	RTN	24
1Ø6	GSB7	23 Ø7	153	+	-55	2ØØ	*LBL3	21 Ø3
1Ø7	RCL4	36 Ø4	154	÷	-24	2Ø1	RCL4	36 Ø4
1Ø8	RCL2	36 Ø2	155	CHS	-22	2Ø2	RCL6	36 Ø6
1Ø9	SIN	41	156	1	Ø1	2Ø3	÷	-24
11Ø	x	-35	157	+	-55	2Ø4	X^2	53
111	GSB4	23 Ø4	158	√X	54	2Ø5	3	Ø3
112	RCL5	36 Ø5	159	RCL5	36 Ø5	2Ø6	x	-35
113	PRTX	-14	16Ø	x	-35	2Ø7	4	Ø4
114	RCL6	36 Ø6	161	GSB4	23 Ø4	2Ø8	÷	-24
115	RCL2	36 Ø2	162	RCLI	36 46	2Ø9	RTN	24
116	SIN	41	163	GSB5	23 Ø5	210	*LBL4	21 Ø4
117	x	-35	164	RTN	24	211	DSP4	-63 Ø4
118	PRTX	-14	165	*LBLD	21 14	212	PRTX	-14
119	SPC	16-11	166	GSB6	23 Ø6	213	RTN	24
12Ø	RCL2	36 Ø2	167	RCL4	36 Ø4	214	*LBL5	21 Ø5
121	GSB5	23 Ø5	168	GSB4	23 Ø4	215	DSP2	-63 Ø2
122	RTN	24	169	RCL6	36 Ø6	216	PRTX	-14

Apparent Crystal Parameters (Concluded)

217	RTN	24	22Ø	*LBL7	21 Ø7	223	RTN	24
218	*LBL6	21 Ø6	221	SPC	16-11	224	R/S	51
219	SPC	16-11	222	SPC	16-11			

Ames Research Center
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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

$a = b = c$
$\alpha = \beta = \gamma = 90°$

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

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

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

Crystal system: Tetragonal

$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

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

$$b \qquad \cos\phi = \frac{\frac{1}{a^2}(h_1h_2 + k_1k_2) + \frac{1}{c^2}(l_1l_2)}{\sqrt{\left[\frac{1}{a^2}(h_1^2 + k_1^2) + \frac{1}{c^2}l_1^2\right]\left[\frac{1}{a^2}(h_2^2 + k_2^2) + \frac{1}{c^2}l_2^2\right]}}$$

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

Crystal system: Orthorhombic

$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

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

$$b \qquad \cos\phi = \frac{\frac{1}{a^2}h_1h_2 + \frac{1}{b^2}k_1k_2 + \frac{1}{c^2}l_1l_2}{\sqrt{\left(\frac{1}{a^2}h_1^2 + \frac{1}{b^2}k_1^2 + \frac{1}{c^2}l_1^2\right)\left(\frac{1}{a^2}h_2^2 + \frac{1}{b^2}k_2^2 + \frac{1}{c^2}l_2^2\right)}}$$

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

Crystal system: Hexagonal

$a = b \neq c$
$\alpha = \beta = 90°;\ \gamma = 120°$

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

$$b \qquad \cos\phi = \frac{h_1h_2 + k_1k_2 + \frac{1}{2}(h_1k_2 + k_1h_2) + \frac{3}{4}\frac{a^2}{c^2}l_1l_2}{\sqrt{\left(h_1^2 + k_1^2 + h_1k_1 + \frac{3}{4}\frac{a^2}{c^2}l_1^2\right)\left(h_2^2 + k_2^2 + h_2k_2 + \frac{3}{4}\frac{a^2}{c^2}l_2^2\right)}}$$

$$c \qquad \cos\rho = \frac{u_1u_2 + v_1v_2 - \frac{1}{2}(u_1v_2 + v_1u_2) + \frac{c^2}{a^2}w_1w_2}{\sqrt{\left(u_1^2 + v_1^2 - u_1v_1 + \frac{c^2}{a^2}w_1^2\right)\left(u_2^2 + v_2^2 - u_2v_2 + \frac{c^2}{a^2}w_2^2\right)}}$$

Crystal system: Rhombohedral

$a = b = c$
$\alpha = \beta = \gamma < 120° \neq 90°$

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

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

$a \neq b \neq c$
$\alpha = \gamma = 90° \neq \beta$

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

b
$$\cos\phi = \frac{\frac{1}{a^2} h_1h_2 + \frac{1}{b^2} k_1k_2\sin^2\beta + \frac{1}{c^2} l_1l_2 - \frac{1}{ac}(l_1h_2 + l_2h_1)\cos\beta}{\left(\left(\frac{1}{a^2} h_1^2 + \frac{1}{b^2} k_1^2\sin^2\beta + \frac{1}{c^2} l_1^2 - \frac{2h_1l_1}{ac}\cos\beta\right) \times \left(\frac{1}{a^2} h_2^2 + \frac{1}{b^2} k_2^2\sin^2\beta + \frac{1}{c^2} l_2^2 - \frac{2h_2l_2}{ac}\cos\beta\right)\right)^{1/2}}$$

c
$$\cos\rho = \frac{a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2 + ac(w_1u_2 + u_1w_2)\cos\beta}{\left((a^2u_1^2 + b^2v_1^2 + c^2w_1^2 + 2acu_1w_1\cos\beta) \times (a^2u_2^2 + b^2v_2^2 + c^2w_2^2 + 2acu_2w_2\cos\beta)\right)^{1/2}}$$

Crystal system: Triclinic

$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma$

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

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

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

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

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

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16. Abstract

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.

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