TWO-CIRCLE CALCULATION IN THE HEXAGONAL SYSTEM

A. L. PARSONS, Toronto University, Toronto, Canada.

Recently the writer had occasion to demonstrate to a class the coordinates that must be used to locate the indices $21\overline{3}1$ in a gnomonic projection of a hexagonal crystal, showing that this meant measuring two fundamental units on the positive end of the a_1 axis, one unit to the right parallel with the a_2 axis, and three units in a negative direction parallel to the a_3 axis, with the height of the plane of projection above



FIG. 1. Gnomonic Projection of Beryl showing h/l, k/l and i/l for the faces 1 $\overline{101}$, 21 $\overline{31}$, $\overline{1212}$ and $\overline{1121}$.

the centre of the sphere of projection as the last index of unity. When this was done he noticed that he had located a point which in the terms of Goldschmidt's pp_0 , qp_0 was to be indicated as 41 which is supposed to have the Bravais indices $41\overline{5}1$.

Further observation showed that in every case there is an intimate rela-

tion between Goldschmidt's co-ordinates pp_0 and qp_0 and the Bravais indices *hkil*, which is quite different from what he and all his pupils have thought, for when these indices are given their proper signs and when h > k > i,

 $pp_0 = \frac{h-i}{l} p_0$ where *h* and *i* have different signs

and

$$qp_0 = \frac{k-i}{l} p_0$$

and

$$p_0 = \frac{2}{3}c.$$

In the accompanying gnomonic projection (Figure 1) of some of the common forms found on beryl a graphical determination of p_0 has been made and the indices for the faces $\overline{1121}$, $\overline{1212}$, $1\overline{101}$, and $21\overline{31}$ are indicated as co-ordinates, with the proper signs, in heavy lines, giving in

each case
$$\frac{h}{l} p_0$$
, $\frac{k}{l} p_0$, and $\frac{i}{l} p_0$.

The following table shows the Bravais symbol for each of these faces together with the proper arrangement of the indices to give the coordinates on the three axes.

Bravais	Indices				Co-ordinates			
	a_1	a_2	a_3		a_1	a_2	a_3	
1121	$\frac{\overline{k}}{l}$	$\frac{\overline{l}}{l}$	$\frac{h}{l}$	=	$\overline{1}p_0$	$\overline{1}p_0$	2p0	
1212	$\frac{\overline{k}}{l}$	$\frac{h}{l}$	$\frac{\overline{l}}{l}$	-	$\frac{\overline{1}}{2}p_0$	$\frac{2}{2}p_0$	$\frac{\overline{1}}{2}p_0$	
1101	$\frac{h}{l}$	$\frac{\overline{k}}{l}$	$\frac{i}{l}$	=	$1p_0$	$\overline{1}p_0$	0¢0	
2131	$\frac{k}{l}$	$\frac{i}{l}$	$\frac{h}{l}$	=	2 <i>p</i> 0	$1p_{0}$	3p0	

Inasmuch as we must consider positive and negative indices, and positive and negative axes, a complete calculation for a hexagonal crystal should determine the sign and position of all three of the coordinates for each and every face. To accomplish this, after the unit first or second order pyramid has been selected by means of the information gained from a gnomonic projection, attention must be paid not only to φ and ρ but to the sectant in which the face lies and the positive or negative character of sin 60° which appears as the divisor in securing pp_0 and qp_0 . In order to obtain the proper signs and positions for the co-ordinates, angle φ should be measured clockwise and 60° - φ counterclockwise, in which case φ may be greater than 30° but not greater than 60° .

In the calculations under these conditions $\sin \varphi$, $\sin 60^{\circ}-\varphi$ and $\tan \rho$ are always positive but the divisor in the fundamental equations, $\sin 60^{\circ}$, is positive when the hypothenuse is parallel with the positive end of an *a* axis, and negative when the hypothenuse is parallel with the negative end of an *a* axis.

With the introduction of positive and negative signs for the indices we

find that

$$\stackrel{+}{q}p_{0} = \frac{k-i}{l}p_{0}$$
, and $\bar{q}p_{0} = \frac{\bar{k}-\bar{i}}{l}p_{0}$, and $\stackrel{+}{p}p_{0} = \frac{h-\bar{i}}{l}p_{0}$, and $\bar{p}p_{0} = \frac{\bar{h}-i}{l}p_{0}$.

Our general formulae then become for pyramidal faces

$$\frac{\sin \phi \cdot \tan \rho}{\pm \sin 60^{\circ}} = \pm q p_0 = \frac{(\pm k) - (\pm i)}{l} p_0$$
$$\frac{\sin (60^{\circ} - \phi) \cdot \tan \rho}{\pm \sin 60^{\circ}} = \pm p p_0 = \frac{(\pm k) - (\mp i)}{l} p_0$$

and prisms

$$\frac{\frac{\sin (60^{\circ} - \varphi)}{\pm \sin 60^{\circ}}}{\frac{\sin \varphi}{\mp \sin 60^{\circ}}} = \frac{\pm p}{\mp q} = \frac{(\pm h) - (\mp i)}{(\mp k) - (\mp i)}.$$

The prism $11\overline{20}$ is apparently an anomalous case for the values of p and q are 1 and 0, but where either p or q is zero the other Goldschmidt co-ordinate for a pyramidal face is $(3/2) h \cdot p_0/l$ and in the case of this

prism the co-ordinate 1/0 must be looked upon as (3/2)h/0 from which the indices $11\overline{2}0$ can be readily deduced.

To illustrate the change involved, the mathematical calculations for a single face of each of the following forms on beryl $(10\overline{1}1)$, $(11\overline{2}2)$, $(11\overline{2}1)$ $(21\overline{3}1)$, $(10\overline{1}0)$ and $(21\overline{3}0)$ are given in the following table, using the values of φ and ρ that correspond to the positions of these forms as determined by the Koksharov axial ratios.

In the column devoted to the angle φ the angle V' is given. V' is the angle measured from the zero position of the projection while φ is the angle obtained by subtracting an integral multiple of 60° from V'. With this change in the magnitude of angle φ , and with pp_0 always greater than qp_0 as given in the formulae above, the position of pp_0 and qp_0 in the calculation becomes interchangeable.

Bravais Symbol	$V' \ arphi$	ρ	$\log \sin 60^\circ - \varphi$ $\log \tan \rho$ $\log \sin \varphi$	log \$\$\$0 log \$\$	$pp_0 = \frac{h-i}{l} p_0$ $qp_0 = \frac{k-i}{l} p_0$	ро Ро	$c = \frac{3}{2}p_0$
1101	150°00′ 30°00′	29°57′	969897 976056 969897	952200 952200	+.33264 33264	.33264 .33264	.4989 .4989
T2T2	0°00′ 0°00′	26°31′	943753 969805 $\overline{\infty}$	969805	+.49895 .0000	.33263	. 4989
<u>Τ</u> Τ21	240°00' 0°00'	44°56′	993753 999899 $\overline{\circ}$	999899 ∞	+.99761	. 33254	. 4988
2131	70°53.4′ 10°53.4′	56°44′	987848 018307 927639	012402 052193	-1.3305 + .3326	.33263 .3326	.4989 .4989
2130	70°53.4′ 10°53.4′	90°00′	987848 927639	$\log \frac{p}{q}$ 060209	$\frac{-p}{+q} = \frac{h-i}{k-i}$ -4.0003		
1101	150°00′ 30°00′	90°00′	969847 969897	$\log \frac{p}{q}$ 000000	$\frac{+p}{-q} = \frac{h-i}{k-i}$ -1.0000		

The calculation gives no new determinations of c:a but by using the angles that have been determined by others confirms the value obtained by Koksharov. For comparison the values are given below:

Koksharov	c = 0.498855
Parsons (Arithmetic)	0.498882
Goldschmidt	$0.8643 = 0.4989\sqrt{3}$

There has been much confusion in the treatment of hexagonal crystals by the two circle method because in either the G_1 or G_2 positions a multiplication or division by $\sqrt{3}$ or a multiple thereof is omitted. This is very evident when the Goldschmidt symbols are the same as those of other workers for in that case the value of c has been multiplied by $\sqrt{3}$ to obtain the Goldschmidt c. Where Goldschmidt's c is the same as that of other workers this is not so evident but it shows in his transformation formula

$$pq(G_2) = \frac{p-2q}{3} \cdot \frac{p-q}{3} (G_1)$$

which when multiplied by $\sqrt{3}$ becomes

$$p\sqrt{3} \cdot q\sqrt{3}(G_2) = \frac{p-2q}{\sqrt{3}} \cdot \frac{p-q}{\sqrt{3}} (G_1).$$

While the mathematical calculation of the crystallographic constants in the hexagonal system is quite simple, the theory underlying the equation for a plane in this system in terms of its intercepts, in terms of the co-ordinates for the line which is perpendicular to the plane, and in terms of its directional cosines, is decidedly complex. It is extremely easy to become confused as is illustrated by a tabulation of the values of c/a as given by Goldschmidt in his Winkeltabellen and by Dana in the sixth edition of his System of Mineralogy, as shown in the table below where a single example is given for each type of difference.

It thus becomes evident that a complete revision of the hexagonal system is necessary for a ready interpretation of two-circle measurements, for there is a lack of agreement in the axial ratio or the symbols or both in every hexagonal mineral.

In spite of the confusion that has arisen from the two orientations G_1 and G_2 the fact remains that in his G_1 position Goldschmidt discovered the simplest method, although on an incorrect assumption, of determin-

THE AMERICAN MINERALOGIST

ing graphically the Bravais indices of any face in the crystal after the unit pyramid $10\overline{1}1$ had been selected. In his G_2 position he had the simplest way of determining graphically p_0 and c. Unfortunately after finding that in every other system his co-ordinates could readily be converted into a:b:c and hkl he could not believe that when he had the

	Dana	Go	ldschmidt	
Bery	$\frac{c}{a} \times \sqrt{3}$	-	$\frac{c}{a}$ G ₁	1010 Dana=1010 Goldschmidt
Microsommite	$\frac{c}{a} \times 2\sqrt{3}$	н	$\frac{c}{a}$ G ₁	1010 Dana=1010 Goldschmidt
Breithauptite	$\frac{c}{a} \times \frac{2}{3} \sqrt{3}$	=	$\frac{c}{a}$ G ₁	$10\overline{1}0$ Dana = $10\overline{1}0$ Goldschmidt
Calcite	$\frac{c}{a}$	-	$\frac{c}{a}$ G ₂	1010 Dana=1120 Goldschmidt
Dioptase	$\frac{c}{a} \times 2$	-	$\frac{c}{a}$ G ₂	1010 Dana=1120 Goldschmidt
Millerite	$\frac{c}{a} \times 3$	-	$\frac{c}{a}$ G ₂	1010 Dana=1120 Goldschmidt
Covellite	$\frac{c}{a} \times 1.5$	=	$\frac{c}{a}$ G ₁ *	1010 Dana=1120 Goldschmidt

* Should be G2.

indices determined by others his ratio of c:a was incorrect and that when he accepted the standard ratio of c:a his indices were wrong.

Largely on account of the confusion caused by the G_1 and G_2 positions there has been considerable opposition on the part of some able crystallographers to the two-circle method. It is hoped that this paper may help to lessen this opposition, and serve as a preliminary to a complete revision of the angle tables for hexagonal minerals.

After this paper had been sent in for publication a much simpler method of calculating indices and axial ratios was found. After selecting the first order unit pyramid, making φ not greater than 30° with h > k > i, then

586

$$\cos \varphi \cdot \tan \rho = \frac{h}{l} \cdot \frac{c}{a}$$
$$\cos (60^\circ - \varphi) \cdot \tan \rho = \frac{k}{l} \cdot \frac{c}{a}$$
$$\cos (60^\circ + \varphi) \cdot \tan \rho = \frac{i}{l} \cdot \frac{c}{a}$$

and for prisms

 $\cos \varphi : \cos (60^\circ - \varphi) : \cos (60^\circ + \varphi) = h : k : i.$

This will be taken up in greater detail in a later paper.