# TWO-CIRCLE CALCULATION IN THE HEXAGONAL SYSTEM

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Recently the writer had occasion to demonstrate to a class the co-ordinates that must be used to locate the indices $21\bar{3}1$ 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

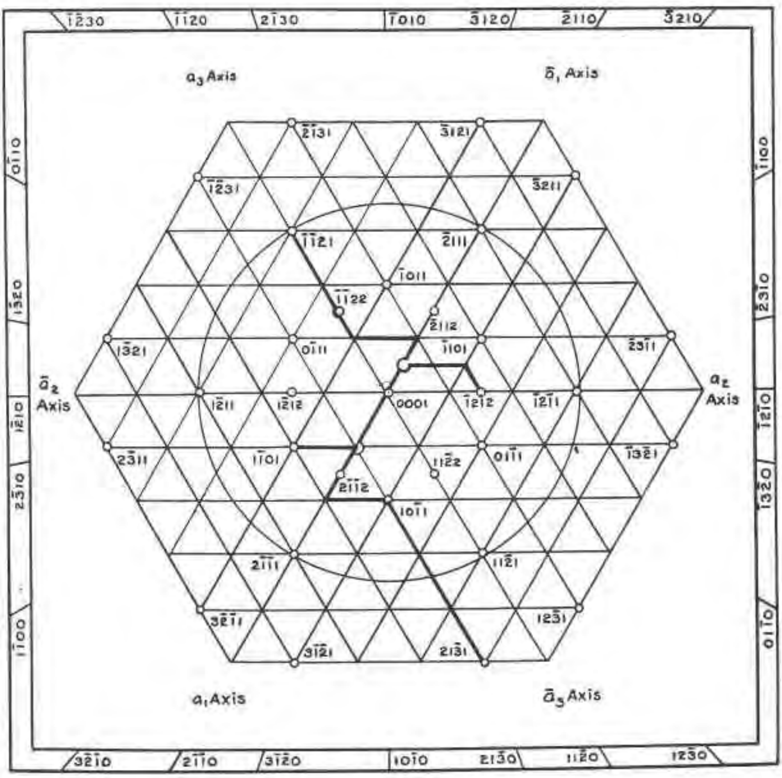


Fig. 1. Gnomonic Projection of Beryl showing $h/l$, $k/l$ and $i/l$ for the faces $1\bar{1}01$, $21\bar{3}1$, $\bar{1}2\bar{1}2$ and $\bar{1}\bar{1}21$.

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 $41\bar{5}1$.

Further observation showed that in every case there is an intimate relation 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 $h>k>i$,

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

and

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

and

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

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 $\bar{1}\bar{1}21$, $\bar{1}2\bar{1}2$, $1\bar{1}01$, and $21\bar{3}1$ 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 co-ordinates on the three axes.

| Bravais | Indices $a_1$ | Indices $a_2$ | Indices $a_3$ | | Co-ordinates $a_1$ | Co-ordinates $a_2$ | Co-ordinates $a_3$ |
|---|---|---|---|---|---|---|---|
| $\bar{1}\bar{1}21$ | $\frac{\bar{k}}{l}$ | $\frac{i}{l}$ | $\frac{h}{l}$ | = | $\bar{1}p_0$ | $\bar{1}p_0$ | $2p_0$ |
| $\bar{1}2\bar{1}2$ | $\frac{\bar{k}}{l}$ | $\frac{h}{l}$ | $\frac{i}{l}$ | = | $\frac{\bar{1}}{2}p_0$ | $\frac{2}{2}p_0$ | $\frac{\bar{1}}{2}p_0$ |
| $1\bar{1}01$ | $\frac{h}{l}$ | $\frac{\bar{k}}{l}$ | $\frac{i}{l}$ | = | $1p_0$ | $\bar{1}p_0$ | $0p_0$ |
| $21\bar{3}1$ | $\frac{k}{l}$ | $\frac{i}{l}$ | $\frac{h}{l}$ | = | $2p_0$ | $1p_0$ | $\bar{3}p_0$ |

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 co-ordinates 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 $\varphi$ and $\rho$ 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 $\varphi$ should be measured clockwise and 60°-$\varphi$ counter-clockwise, in which case $\varphi$ may be greater than 30° but not greater than 60°.

In the calculations under these conditions sin $\varphi$, sin 60°-$\varphi$ and tan $\rho$ are always positive but the divisor in the fundamental equations, sin 60°, 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

$$\overset{+}{q}\,p_0=\frac{k-i}{l}\,p_0,\ \text{and}\ \bar{q}\,p_0=\frac{\bar{k}-\bar{i}}{l}\,p_0,\ \text{and}\ \overset{+}{p}\,p_0=\frac{h-\bar{i}}{l}\,p_0,\ \text{and}\ \bar{p}\,p_0=\frac{\bar{h}-i}{l}\,p_0.$$

Our general formulae then become for pyramidal faces

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

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

and prisms

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

The prism $11\bar{2}0$ 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 $11\bar{2}0$ can be readily deduced.

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

In the column devoted to the angle $\varphi$ the angle $V'$ is given. $V'$ is the angle measured from the zero position of the projection while $\varphi$ is the angle obtained by subtracting an integral multiple of 60° from $V'$. With this change in the magnitude of angle $\varphi$, 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 | $V'$<br>$\varphi$ | $\rho$ | log sin 60° $-\varphi$<br>log tan $\rho$<br>log sin $\varphi$ | log $pp_0$<br>log $qp_0$ | $pp_0=\frac{h-i}{l}p_0$<br>$qp_0=\frac{k-i}{l}p_0$ | $p_0$<br>$p_0$ | $c=\frac{3}{2}p_0$ |
|---|---|---|---|---|---|---|---|
| $1\bar{1}01$ | 150°00′<br>30°00′ | 29°57′ | 969897<br>976056<br>969897 | 952200<br>952200 | +.33264<br>−.33264 | .33264<br>.33264 | .4989<br>.4989 |
| $\bar{1}2\bar{1}2$ | 0°00′<br>0°00′ | 26°31′ | 943753<br>969805<br>$\overline{\infty}$ | 969805<br><br>$\overline{\infty}$ | +.49895<br>.0000 | .33263 | .4989 |
| $\bar{1}\bar{1}21$ | 240°00′<br>0°00′ | 44°56′ | 993753<br>999899<br>$\overline{\infty}$ | 999899<br><br>$\overline{\infty}$ | +.99761<br>.0000 | .33254 | .4988 |
| $21\bar{3}1$ | 70°53.4′<br>10°53.4′ | 56°44′ | 987848<br>018307<br>927639 | 012402<br>052193 | −1.3305<br>+ .3326 | .33263<br>.3326 | .4989<br>.4989 |
| $21\bar{3}0$ | 70°53.4′<br>10°53.4′ | 90°00′ | 987848<br>—<br>927639 | log $\frac{p}{q}$<br><br>060209 | $\frac{-p}{+q}=\frac{h-i}{k-i}$<br><br>−4.0003 | | |
| $1\bar{1}01$ | 150°00′<br>30°00′ | 90°00′ | 969847<br>—<br>969897 | log $\frac{p}{q}$<br><br>000000 | $\frac{+p}{-q}=\frac{h-i}{k-i}$<br><br>−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 determining graphically the Bravais indices of any face in the crystal after the unit pyramid $10\bar{1}1$ 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 | | Goldschmidt | |
|---|---|---|---|---|
| Bery | $\frac{c}{a}\times\sqrt{3}$ | = | $\frac{c}{a}$ $G_1$ | $10\bar{1}0$ Dana $= 10\bar{1}0$ Goldschmidt |
| Microsommite | $\frac{c}{a}\times 2\sqrt{3}$ | = | $\frac{c}{a}$ $G_1$ | $10\bar{1}0$ Dana $= 10\bar{1}0$ Goldschmidt |
| Breithauptite | $\frac{c}{a}\times\frac{2}{3}\sqrt{3}$ | = | $\frac{c}{a}$ $G_1$ | $10\bar{1}0$ Dana $= 10\bar{1}0$ Goldschmidt |
| Calcite | $\frac{c}{a}$ | = | $\frac{c}{a}$ $G_2$ | $10\bar{1}0$ Dana $= 11\bar{2}0$ Goldschmidt |
| Dioptase | $\frac{c}{a}\times 2$ | = | $\frac{c}{a}$ $G_2$ | $10\bar{1}0$ Dana $= 11\bar{2}0$ Goldschmidt |
| Millerite | $\frac{c}{a}\times 3$ | = | $\frac{c}{a}$ $G_2$ | $10\bar{1}0$ Dana $= 11\bar{2}0$ Goldschmidt |
| Covellite | $\frac{c}{a}\times 1.5$ | = | $\frac{c}{a}$ $G_1$* | $10\bar{1}0$ Dana $= 11\bar{2}0$ Goldschmidt |

* Should be $G_2$.

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 $\varphi$ not greater than 30° with $h>k>i$, then

$$\cos \varphi \cdot \tan \rho = \frac{h}{l} \cdot \frac{c}{a}$$

$$\cos (60° - \varphi) \cdot \tan \rho = \frac{k}{l} \cdot \frac{c}{a}$$

$$\cos (60° + \varphi) \cdot \tan \rho = \frac{i}{l} \cdot \frac{c}{a}$$

and for prisms

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

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