CALCULATION OF POLAR AND DIRECT AXIAL RATIOS AND POLAR AND DIRECT AXIAL ANGLES OF TRICLINIC CRYSTALS FROM INTERFACIAL ANGLES

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ABSTRACT

The polar axial ratios of a triclinic crystal can be calculated by means of the equations:

$$\frac{p_0'}{r_0'} = \frac{l \sin (001 \wedge h0l)}{h \sin (100 \wedge h0l)}, \tag{1'}$$

$$\frac{q_0'}{r_0'} = \frac{l \sin (001 \wedge 0kl)}{k \sin (010 \wedge 0kl)}, \tag{2'}$$

and

$$\frac{p_0'}{q_0'} = \frac{k \sin (010 \wedge hk0)}{h \sin (100 \wedge hk0)}. \tag{3'}$$

The polar axial ratios of some triclinic minerals can thus be obtained as the ratios of the sines of measured interfacial angles. The polar axial angles λ, μ, and ν of a triclinic crystal are by definition the interfacial angles 010∧001, 100∧001, and 100∧010 respectively. The polar axial angles of some triclinic minerals can thus be obtained as measured interfacial angles or as the sums of measured interfacial angles. In the absence of one or more of the necessary faces it will be impossible to measure one or more of the interfacial angles needed for the application of at least two of the equations (1'), (2'), and (3'). The required interfacial angles can then be calculated from measured interfacial angles in some cases by the methods of plane trigonometry, in other cases only by the methods of spherical trigonometry, provided at least 5 interfacial angles have been measured that will permit the solution of certain triangles.

The direct axial ratios of triclinic crystals can be evaluated as the ratios of the sines of certain interzonal angles, as is well known. These interzonal angles are not equal to any interfacial angles in the case of triclinic crystals, but they can be calculated from certain interfacial angles by the methods of spherical trigonometry, and this has been the practice of crystallographers making use of the one-circle goniometer or the contact-hand-goniometer.

The direct axial ratios of triclinic crystals can be calculated more easily in many cases by means of the polar axial ratios and polar axial angles than by means of interzonal angles. The equations necessary for this purpose are derived very simply by the application of the law of sines for spherical oblique triangles.

A simple method of calculation of crystallographic axial ratios and axial angles, and a simple method of determination of Miller indices from measurements of interfacial angles with the one-circle goniometer or with the contact goniometer, are especially needed by mineralogists and geologists whose principal interests are in branches of geologic science other than crystallography but who wish to make some use of crystallographic data in mineral determination. The purpose of this paper is to outline the simplest methods known to the writer of accomplishing these results.

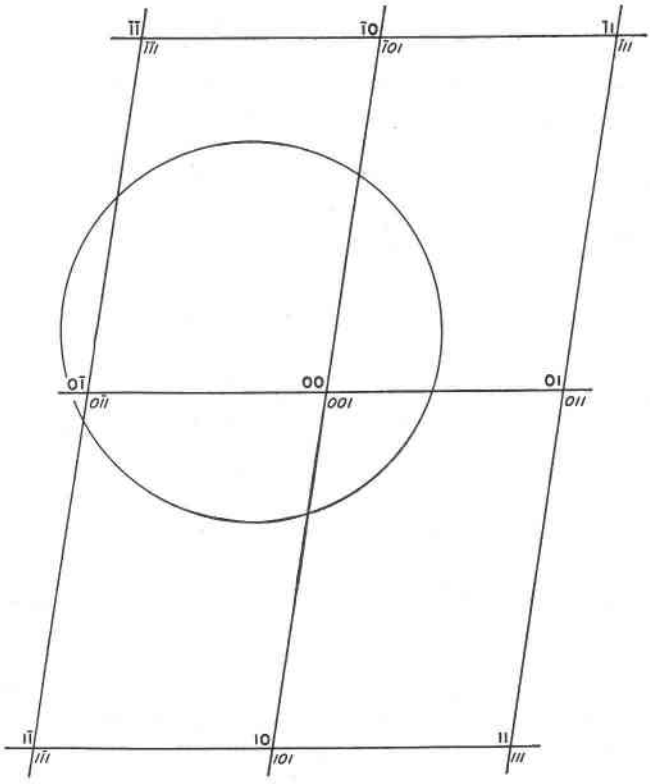

FIG. 1. Gnomonic projection of a triclinic crystal. The figures in roman type are the coordinates in the plane of the gnomonic projection; the figures in italics are the Miller indices.

The Miller indices of crystal faces can usually be determined most easily by the use of the gnomonic projection (Fig. 1) and the polar lattice.[1] This method of indexing faces has been the usual procedure in cases of measurements of coordinate angles by means of the two-circle goniometer, and, as T. V. Barker[2] has pointed out, it can also be readily applied with measurements of interfacial angles by means of the one-circle goniometer or contact goniometer. In order to determine the Miller indices of a face by this method from measurements of interfacial angles, it is best to construct the stereographic pole of the face by the use of a

[1] The polar lattice of the mineralogist is identical in proportions and angles with the reciprocal lattice of the x-ray crystallographer, but is not, in general, drawn to the same scale (Palache, C. *Am. Mineral.*, **19**, 108 (1934)).

[2] Barker, T. V. Graphical and Tabular Methods in Crystallography, Thomas Murby & Co., London, 1922, p. 25.

stereonet and then to construct the gnomonic pole from the stereographic pole by means of an auxiliary section (Fig. 2) or by the use of a stereographic-gnomonic protractor. Application of Neumann's gnomonic theorem then permits the indices of the face to be obtained from the

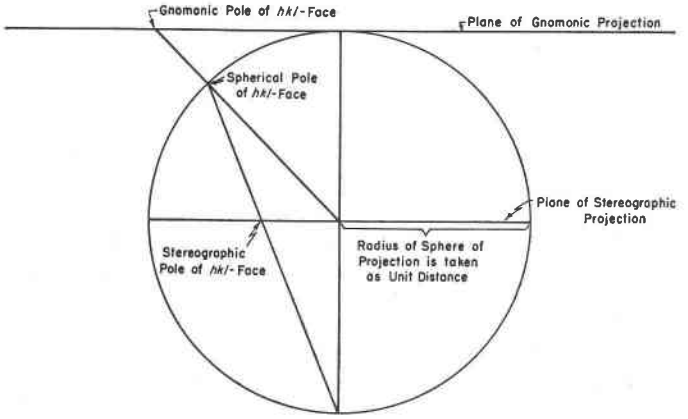

FIG. 2. Construction of the gnomonic pole of a face from its stereographic pole in the case of a triclinic crystal.

coordinates of the gnomonic pole, provided the plane of the gnomonic projection is parallel to two of the polar axes, by the addition of the third coordinate, which is one, and the multiplication of all three coordinates by the smallest factor necessary to convert all fractions, if there are any fractions, into integers. The plane of the gnomonic projection being coincident with the first level of the polar lattice, the face-poles in the gnomonic projection the coordinates of which are integers are nodes of the first level of the polar lattice (Fig. 3); face-poles in the gnomonic projection having one or both coordinates fractional correspond to nodes of higher levels of the polar lattice projected onto the gnomonic plane along the face-normals.

In all crystal systems the polar axial angles are defined as the angles between the edges of a parallelepiped constructed with its edges perpendicular to the faces 100, 010, and 001, and with its body diagonal perpendicular to the face 111, and the polar axial ratios are defined as the ratios of the lengths of the edges of this parallelepiped. The edge perpendicular to the face 100 is designated p_0' in this paper, the edge perpendicular to the face 010 is designated q_0', and the edge perpendicular to the face 001 is designated r_0'; the angle between q_0' and r_0' is designated λ, the angle between p_0' and r_0' is designated μ, and the angle between p_0' and q_0' is designated ν. The polar axial angle λ is thus by

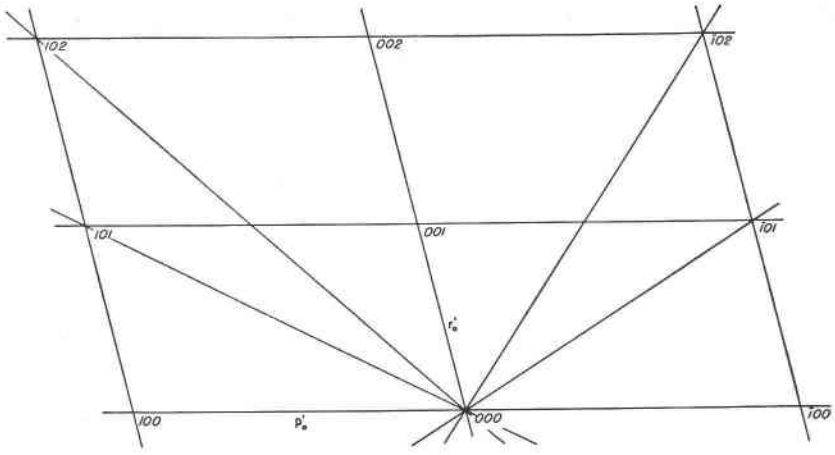

FIG. 3. Section of the polar lattice of a triclinic crystal through the normals to 100 and 001.

definition the angle between the normals to the faces 010 and 001. Likewise the polar axial angle μ is by definition the angle between the normals to the faces 100 and 001, and the polar axial angle ν is by definition the angle between the normals to the faces 100 and 010.

The fundamental relations between polar axial ratios and interfacial angles can be derived very easily. In Fig. 4 let OA represent a line perpendicular to the face 100, OB a line perpendicular to the face 010, and OM a line perpendicular to the face 110 of a triclinic crystal. Then, by

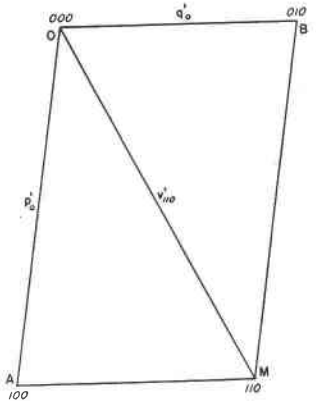

FIG. 4. Relationship of the polar lattice elements p_0' and q_0' of a triclinic crystal to the interfacial angles $100 \wedge 110$ and $010 \wedge 110$.

applying the law of sines for plane triangles to the triangle OBM, we obtain immediately the relation

$$\frac{p_0'}{q_0'} = \frac{\sin \angle BOM}{\sin \angle OMB} = \frac{\sin (010 \wedge 110)}{\sin (100 \wedge 110)}.^3 \qquad (1)$$

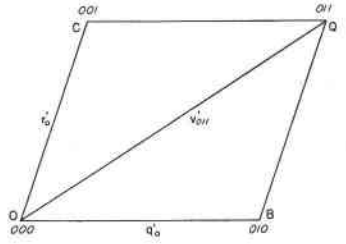

FIG. 5. Relationship of the polar lattice elements q_0' and r_0' of a triclinic crystal to the interfacial angles 010∧011 and 001∧011.

In Fig. 5 let OB represent a line perpendicular to the face 010, OC a line perpendicular to the face 001, and OQ a line perpendicular to the face 011. By applying the law of sines for plane triangles to the triangle OBQ, we obtain the relation

$$\frac{q_0'}{r_0'} = \frac{\sin \angle OQB}{\sin \angle BOQ} = \frac{\sin (001 \wedge 011)}{\sin (010 \wedge 011)}. \qquad (2)$$

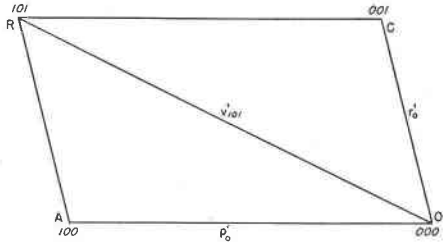

FIG. 6. Relationship of the polar lattice elements p_0' and r_0' of a triclinic crystal to the interfacial angles 100∧101 and 001∧101.

In Fig. 6 let OA represent a line perpendicular to the face 100, OC a line perpendicular to the face 001, and OR a line perpendicular to the face 101. By applying the law of sines for plane triangles to the triangle OCR, we obtain the relation

[3] Goldschmidt, V. Einleitung in die formbeschreibende Krystallographie, Julius Springer, Berlin, 1887, p. 102.

$$\frac{p_0'}{r_0'} = \frac{\sin \angle COR}{\sin \angle CRO} = \frac{\sin (001 \wedge 101)}{\sin (100 \wedge 101)}. \tag{3}$$

Thus, the polar axial ratios can be calculated from the four interfacial angles 100∧010, 100∧001, 100∧101, 100∧110, or from the four interfacial angles 100∧010, 001∧010, 100∧110, 010∧011, or from the four interfacial angles 100∧001, 010∧001, 100∧101, 010∧011 in the most general case, that of the triclinic system.

If the face 110 is not present on the crystal, but some face $hk0$ is present in the zone containing the faces 100 and 010, the ratio of p_0' to q_0' can be obtained by the use of the equation

$$\frac{hp_0'}{kq_0'} = \frac{\sin (010 \wedge hk0)}{\sin (100 \wedge hk0)}. \tag{1'}$$

Likewise, if the face 011 is not present on the crystal, but some face $0kl$ is present in the zone containing the faces 010 and 001, the ratio of q_0' to r_0' can be obtained by the use of the equation

$$\frac{kq_0'}{lr_0'} = \frac{\sin (001 \wedge 0kl)}{\sin (010 \wedge 0kl)}. \tag{2'}$$

Similarly, if the face 101 is not present on the crystal, but some face $h0l$ is present in the zone containing the faces 100 and 001, the ratio of p_0' to r_0' can be obtained by the use of the equation

$$\frac{hp_0'}{lr_0'} = \frac{\sin (001 \wedge h0l)}{\sin (100 \wedge h0l)}. \tag{3'}$$

Hence if the forms {100}, {010}, {001}, and either one $\{h0l\}$-form and one $\{0kl\}$-form, or one $\{h0l\}$-form and one $\{hk0\}$-form, or one $\{0kl\}$-form and one $\{hk0\}$-form are present on the crystal, all the polar axial ratios and polar axial angles of a triclinic crystal can be obtained by the measurement of five interfacial angles and the calculation of two quotients of sines of measured angles. One or another of these combinations of forms is a combination of common forms of the following triclinic minerals: babingtonite, amblygonite, wollastonite, axinite, and tarbuttite, and this method could thus be used to calculate the polar axial ratios and polar axial angles of crystals of these minerals.

If various other combinations of forms are present, the calculation of all the polar axial ratios and polar axial angles of a triclinic crystal can still be accomplished very simply by the application of the equations of plane trigonometry. This is possible, for example, if the forms {001} and {010} and two $\{hk0\}$-forms, one $\{0kl\}$-form, and one $\{h0l\}$-form are present (a combination of forms that is commonly found on triclinic as well as on monoclinic feldspar crystals).

It is not possible, of course, to calculate all the polar axial ratios and polar axial angles from measured interfacial angles of triclinic crystals

in all cases without the solution of any spherical triangle. Thus, for example, if only the forms {100}, {010}, {110}, {011}, {0$\bar{1}$1} were present, it would be necessary to solve two oblique spherical triangles in order to calculate all the polar axial ratios and polar axial angles[4] from measurements of the interfacial angles.[5]

The direct crystallographic elements of a triclinic crystal are the interaxial angles, α, β, γ, and the axial ratios, a/b and c/b. The direct axial ratios and axial angles can be calculated from the interfacial angles; in some cases, however, the direct axial ratios can be calculated more easily from the polar axial ratios and polar axial angles.

The derivation of the equations needed for the calculation of the direct crystallographic elements of a triclinic crystal from measurements of interfacial angles has been given in several treatises[6] and is as follows.

[4] Since only the relative dimensions of the polar lattice are fixed by measurements of interfacial angles, the scale on which the polar lattice is drawn in morphological work is arbitrary. In investigations of crystals with the two-circle goniometer, the plane of the gnomonic projection has been constructed tangent to the projection sphere, the length of the radius of this sphere being taken equal to unity. Elements of the polar lattice drawn on this scale have been called "projection elements" by V. Goldschmidt and those who have made use of his methods of calculation, and have been designated by letters with primes by them. Elements of the polar lattice drawn on the smaller scale on which the length of the element normal to the face 001 is taken as equal to unity have been called "polar elements" by Goldschmidt and those who have made use of his methods, and have been designated by letters with subscript zeros by them. In this paper, where the scale is that of the "projection elements," the phrase "polar lattice elements" is used rather than "polar elements," since, in the terminology of Goldschmidt and those who have made use of his methods, "polar elements" are based on the scale on which the length of the element normal to the face 001 is taken as equal to unity. It is clear, however, that both Goldschmidt's "projection elements" and his "polar elements" are elements of polar lattices that differ only in scale.

[5] As Barker and others have stated, greater accuracy is usually obtainable with measurements of coordinate angles made by means of a two-circle goniometer than with measurements of interfacial angles made by the use of a one-circle goniometer. In the investigation of complex crystals there is also an important saving of time and labor when the two-circle goniometer is used. The very simple fundamental relations between interfacial angles and polar elements as well as the simple fundamental relations between interzonal angles and direct elements need to be understood by students of mineralogy, however, even if they intend to proceed to the more complicated methods permitting the calculation of the most accurate values of the crystallographic elements from measurements of the coordinate angles with the two-circle goniometer. Moreover, measurements of interfacial angles made with the one-circle goniometer or with the contact goniometer are important in determinative work.

[6] Cf. Liebisch, T., Grundriss der physikalischen Krystallographie, Veit & Comp., Leipzig, 1896, pp. 21–22, Tutton, A. E. H., Crystallography and Practical Crystal Measurement, Macmillan and Co., London, 1922, Vol. 1, p. 111, Peacock, M. A., in Technique of Organic Chemistry, Edited by A. Weissberger, Interscience Publishers, New York, 1949, Vol. 1, Second Edition, Part 1, pp. 1005–1006.

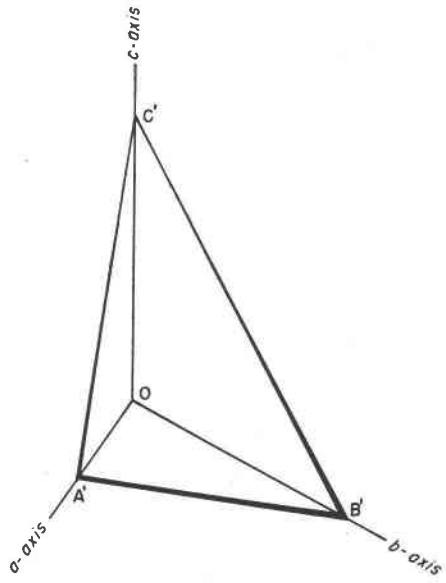

FIG. 7. Relationship of the unit plane 111 to the unit distances along the a-axis, b-axis, and c-axis in the case of a triclinic crystal.

In Fig. 7 the plane $A'B'C'$ represents the plane chosen as the unit plane 111. The ratios of its intercepts on the three crystallographic axes are consequently the axial ratios, that is,

$$\frac{\overline{OA'}}{\overline{OB'}} = \frac{a}{b} \tag{4}$$

and

$$\frac{\overline{OC'}}{\overline{OB'}} = \frac{c}{b}. \tag{5}$$

By applying the law of sines for plane triangles to the triangle $OA'B'$, one obtains immediately

$$\frac{\overline{OA'}}{\sin \angle OB'A'} = \frac{\overline{OB'}}{\sin \angle OA'B'}, \tag{6}$$

and, combining equations (4) and (6), one has

$$\frac{a}{b} = \frac{\sin \angle OB'A'}{\sin \angle OA'B'}. \tag{7}$$

Now the angle $OB'A'$ is the angle between the zone-axis OB' (which is the zone-axis of the zone including 100 and 001) and the zone-axis $A'B'$ (which is the zone-axis of the zone including 111 and 001). Also

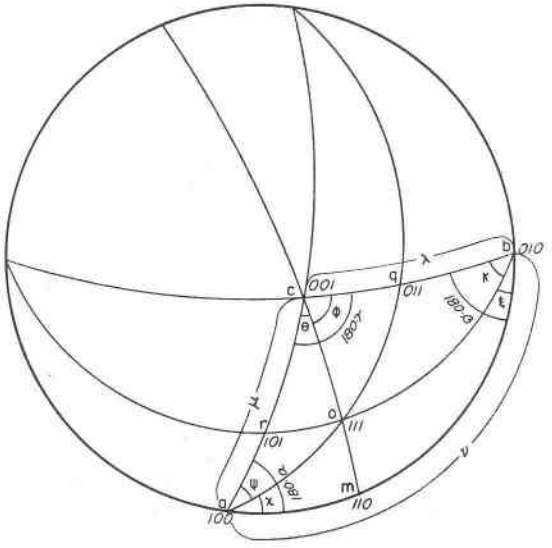

FIG. 8. Relationships of the principal interfacial and interzonal angles in the stereographic projection of a triclinic crystal. The points *a*, *b*, and *c* are the stereographic poles of the faces 100, 010, and 001 respectively (the points *a*, *b*, and *c* are not the stereographic projections of the points in which the *a*-axis, *b*-axis, and *c*-axis intersect the sphere of projection in the case of a triclinic crystal). The *a*-axis, *b*-axis, and *c*-axis are not drawn in the figure; they are perpendicular to the great circles *bqc*, *cra*, and *amb* respectively.

the angle θ in the stereographic projection of the crystal faces (Fig. 8) is the angle between the zone including 100 and 001 and the zone including 111 and 001. Therefore $\theta = \angle OB'A'$. Furthermore the angle $OA'B'$ is the angle between the zone-axis OA' (which is the zone-axis of the zone including 010 and 001) and the zone-axis $B'A'$ (which is the zone-axis of the zone including 111 and 001). And, the angle ϕ in the stereographic projection (Fig. 8) is the angle between the zone including 010 and 001 and the zone including 111 and 001. Therefore $\phi = \angle OA'B'$. Hence, by substituting $\sin\theta$ for $\sin \angle OB'A'$ and $\sin\phi$ for $\sin \angle OA'B'$ in equation (7), one obtains

$$\frac{a}{b} = \frac{\sin\theta}{\sin\phi}. \tag{8}$$

Similarly, by applying the law of sines for plane triangles to the triangle $OB'C'$, one obtains

$$\frac{\overline{OC'}}{\sin \angle OB'C'} = \frac{\overline{OB'}}{\sin \angle OC'B'}, \tag{9}$$

and combining equations (5) and (9), one has

$$\frac{c}{b} = \frac{\sin \angle OB'C'}{\sin \angle OC'B'}. \tag{10}$$

Now the angle $OB'C'$ is the angle between the zone-axis OB' (which is the zone-axis of the zone including 100 and 001) and the zone-axis $C'B'$ (which is the zone-axis of the zone including 100 and 111). Also the angle ψ in the stereographic projection (Fig. 8) is the angle between the zone including 100 and 001 and the zone including 100 and 111. Therefore $\psi = \angle OB'C'$. Furthermore the angle $OC'B'$ is the angle between the zone including 100 and 010 and the zone including 100 and 111. And the angle χ in the stereographic projection (Fig. 8) is the angle between the zone including 100 and 010 and the zone including 100 and 111. Therefore $\chi = \angle OC'B'$. Hence, by substituting $\sin \psi$ for $\sin \angle OB'C'$ and $\sin \chi$ for $\sin \angle OC'B'$ in equation (10), one obtains

$$\frac{c}{b} = \frac{\sin \psi}{\sin \chi}. \tag{11}$$

By means of equations (8) and (11) the direct axial ratios of a triclinic crystal can be calculated from the interzonal angles θ, ϕ, ψ, and χ. These interzonal angles must themselves be calculated from the measured interfacial angles by application of the equation of spherical trigonometry giving the angle of an oblique spherical triangle in terms of the three sides.

The interaxial angles, α, β, γ, of a triclinic crystal are the supplements of the angles of the spherical triangle abc (Fig. 8),

$$\alpha = 180° - \angle bac, \tag{12}$$

$$\beta = 180° - \angle abc, \tag{13}$$

$$\gamma = 180° - \angle acb. \tag{14}$$

Thus α, β, and γ can be calculated from the measurements of the interfacial angles $100 \wedge 010$, $100 \wedge 001$, and $010 \wedge 001$, which are the sides of this spherical triangle. By applying the standard formula of spherical trigonometry giving an angle of an oblique spherical triangle in terms of the three sides[7] one obtains

$$\sin \frac{\angle bac}{2} = \sqrt{\frac{\sin (s-\mu) \sin (s-\nu)}{\sin \mu \sin \nu}}, \tag{15}$$

where $s = (\lambda + \mu + \nu)/2$. Hence, making use of equation (12), one has

$$\sin \frac{180° - \alpha}{2} = \sqrt{\frac{\sin (s-\mu) \sin (s-\nu)}{\sin \mu \sin \nu}} \tag{16}$$

and, finally,

[7] This standard formula is to be found in text-books of spherical trigonometry.

$$\cos\frac{\alpha}{2} = \sqrt{\frac{\sin(s-\mu)\sin(s-\nu)}{\sin\mu\sin\nu}}. \tag{17}$$

In an analogous way one can prove that

$$\cos\frac{\beta}{2} = \sqrt{\frac{\sin(s-\lambda)\sin(s-\nu)}{\sin\lambda\sin\nu}} \tag{18}$$

and

$$\cos\frac{\gamma}{2} = \sqrt{\frac{\sin(s-\lambda)\sin(s-\mu)}{\sin\lambda\sin\mu}}. \tag{19}$$

Instead of calculating the direct axial ratios of a triclinic crystal from interfacial angles, one can compute them more easily in some cases from the polar axial ratios and polar axial angles by means of the well known equations[8]

$$\frac{a}{b} = \frac{q_0'\sin\lambda}{p_0'\sin\mu}, \tag{20}$$

and

$$\frac{c}{b} = \frac{q_0'\sin\nu}{r_0'\sin\mu}. \tag{21}$$

These equations can be readily derived by application of the law of sines for oblique spherical triangles. In Fig. 8 the angle *am* is the angle between the face 100 and the face 110,

$$\angle am = 100 \wedge 110, \tag{22}$$

also the angle *mb* is the angle between the face 110 and the face 010,

$$\angle mb = 110 \wedge 010. \tag{23}$$

Applying the law of sines for oblique spherical triangles to the triangle *amc*, one obtains

$$\frac{\sin\theta}{\sin\angle am} = \frac{\sin\angle amc}{\sin\angle ac} \tag{24}$$

and applying the same law to the triangle *bmc*, one obtains

$$\frac{\sin\phi}{\sin\angle mb} = \frac{\sin\angle bmc}{\sin\angle bc}. \tag{25}$$

Now $\angle amc + \angle bmc = 180°$, since *amb* is an arc of a great circle. Therefore

$$\sin\angle amc = \sin\angle bmc. \tag{26}$$

Substituting this value for $\sin\angle bmc$ in equation (25), one obtains

[8] Cf. Palache, C., *Am. Mineral.*, **5**, 81 (1920), Goldschmidt, V., Kursus der Kristallometrie, Gebrüder Borntraeger, Berlin, 1934, p. 135, Hermann, C., Editor, Internationale Tabellen zur Bestimmung von Kristallstrukturen, Bd. 1, Gebrüder Borntraeger, Berlin, 1935, p. 68.

$$\frac{\sin\theta}{\sin\angle am}\sin\angle ac = \sin\angle amc = \frac{\sin\phi}{\sin\angle mb}\sin\angle bc. \tag{27}$$

Since $\angle am = 100 \wedge 110$ and $\angle mb = 110 \wedge 010$ and $\angle ac = \mu$ and $\angle bc = \lambda$, we have

$$\frac{\sin\theta}{\sin\phi} = \frac{\sin\lambda}{\sin\mu}\frac{\sin(100 \wedge 110)}{\sin(010 \wedge 110)}, \tag{28}$$

and, making use of equations (1) and (8), one obtains finally

$$\frac{a}{b} = \frac{q_0'}{p_0'}\frac{\sin\lambda}{\sin\mu}.^{9} \tag{29}$$

Equation (21) is readily derived in an analogous way.

Acknowledgment

The author is indebted to the late Dr. F. E. Wright and to Professor Joseph Murdoch for kindly reading the manuscript of this paper and offering constructive suggestions.

[9] Equations (20) and (21) can be derived very simply from the definitions of the reciprocal lattice vectors. The derivation given in this paper can, however, be used by those who have not studied the methods of vector analysis, and may also be of value to mineralogists who are familiar with the derivation by means of vectors, since it brings out certain fundamental morphological relations.

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