

# RELATIONS AMONG CRYSTALLOGRAPHIC ELEMENTS

HOWARD T. EVANS, JR.,

*Section of Graphics, Massachusetts Institute of Technology.*

## ABSTRACT

Explicit formulae are given relating the three sets of morphological elements for the triclinic system: axial, projection and polar elements.

It has become customary, when reporting morphological data in the literature, to record the values of certain characteristic constants or elements. For a triclinic crystal, the most general case, there are five, and these are customarily computed in three different ways. This process yields the axial elements ( $a$ ,  $c$ ,  $\alpha$ ,  $\beta$ , and  $\gamma$ ), the projection elements ( $x_0'$ ,  $y_0'$ ,  $p_0'$ ,  $q_0'$ , and  $\nu$ ), and the polar elements ( $p_0$ ,  $q_0$ ,  $\lambda$ ,  $\mu$ , and  $\nu$ ). While all these values are given in modern references (such as the 7th edition of

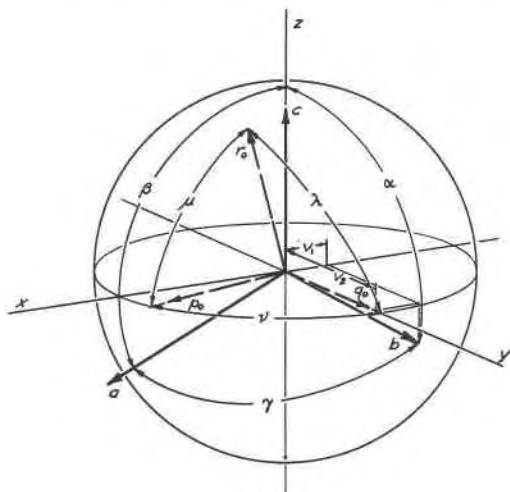


FIG. 1. Triclinic axes and angles.

*Dana's System of Mineralogy*), the larger proportion of data in the literature provides only the axial elements, especially with respect to artificial compounds. Naturally, each element is explicitly expressible in terms of the elements of any other set; such expressions would enable the crystallographer to transform from one set to another at his convenience. These relationships have been derived and found very useful in this laboratory. Since they do not appear to be published together anywhere, at least within easy reach, it seems worthwhile to record them here.

The elements listed above are described by means of two sketches, Fig. 1 and Fig. 2. For further definitions and relations, see the Introduc-

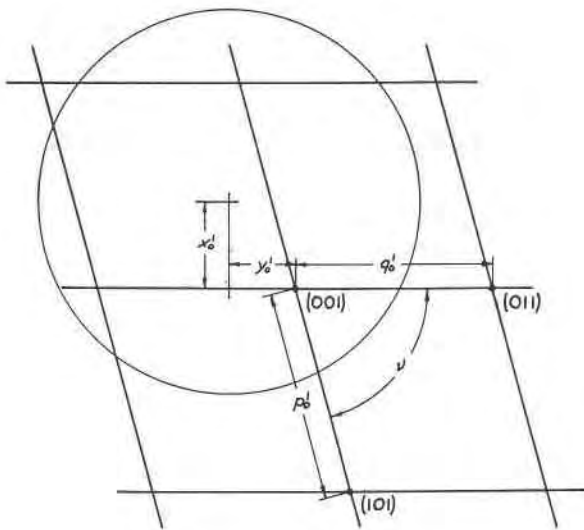


FIG. 2. Triclinic gnomonic projection.

tion to the *System*.<sup>1</sup> Two additional constants are of great value in these formulae. These are the components  $v_1$  and  $v_2$  of the unit  $b$ -axis on the  $x$ - and  $y$ -axes of Cartesian coordinates, respectively. The most useful transformation formulae are collected in Table 1.

TABLE 1. TRANSFORMATION FORMULAE AMONG THE THREE SETS OF TRICLINIC ELEMENTS

$$(1) \quad v_1 = \frac{\cos \gamma - \cos \alpha \cos \beta}{\sin \beta}$$

$$(2) \quad v_2 = \frac{\sqrt{1 + 2 \cos \alpha \cos \beta \cos \gamma - (\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma)}}{\sin \beta}$$

$$(3) \quad v_1 = -\frac{\cos \nu}{\sqrt{1 + (x_0' \cos \nu - y_0' \sin \nu)^2}}$$

$$(4) \quad v_2 = \frac{\sin \nu}{\sqrt{1 + (x_0' \cos \nu - y_0' \sin \nu)^2}}$$

Axial elements:

$$(5) \quad a = \frac{q_0' v_2 \sqrt{1 + x_0'^2}}{p_0' \sin \nu}$$

$$(6) \quad c = q_0' v_2$$

$$(7) \quad \cot \alpha = x_0' \cos \nu - y_0' \sin \nu^2$$

$$(8) \quad \cot \beta = -x_0'$$

$$(9) \quad \cos \gamma = \frac{v_1 + x_0'(v_1 x_0' + v_2 y_0')}{\sqrt{1 + x_0'^2}}$$

<sup>1</sup> Palache, Berman and Frondel, *Dana's System of Mineralogy*, 7th ed., pp. 3-37; John Wiley & Sons, Inc., New York (1944). This section is reprinted from C. W. Wolfe, *Am. Mineral.*, **26**, 55-91 (1941).

<sup>2</sup> The relation:  $\sin \alpha = \sqrt{v_1^2 + v_2^2}$ , is also useful, but is not used in this list because of the ambiguity with regard to the quadrant of  $\alpha$ .

TABLE 1—(continued)

Projection elements:

$$(10) \quad x_0' = -\cot$$

$$(11) \quad y_0' = \frac{v_1 \cot \beta - \cos \alpha}{v_2}$$

$$(12) \quad p_0' = \frac{c \sin \alpha}{av_2 \sin \beta}$$

$$(13) \quad q_0' = \frac{c}{v_2}$$

$$(14) \quad \tan \nu = -\frac{v_2}{v_1}$$

Polar elements:

$$(15) \quad r_0' = \sqrt{x_0'^2 + y_0'^2 + 1}$$

$$(16) \quad p_0 = \frac{p_0'}{r_0'}$$

$$(17) \quad q_0 = \frac{q_0'}{r_0'}$$

$$(18) \quad \cos \lambda = \frac{y_0'}{r_0'} = y_0$$

$$(19) \quad \cos \mu = \frac{x_0'v_2 - y_0'v_1}{r_0'\sqrt{v_1^2 + v_2^2}}$$

$$(20) \quad \tan \nu = -\frac{v_2}{v_1}$$

By appropriate substitution of  $\alpha = \gamma = 90^\circ$ , these formulae may be rewritten for the monoclinic system. Thus,  $v_2 = 1$  and  $v_1$  vanishes. The results are so greatly simplified that they may be written down at once by inspection of Table 1. The remaining systems become trivial.

The constants  $v_1$  and  $v_2$  are seen to be very useful in the expression of these formulae. They are so much so in all calculations in this system that the first step in any study of a triclinic crystal, once a particular orientation is chosen, should be their evaluation. It is therefore urged that  $v_1$  and  $v_2$  be included in the description of a triclinic crystal, even at the risk of increasing the bulk of data already recorded for this system.

Very briefly, the best approach to these formulae is described as follows. W. L. Bond<sup>3</sup> has expressed the components of the triclinic axes on the axes of Cartesian coordinates in terms of a matrix:

$$M = \begin{vmatrix} a \sin \beta & v_1 & 0 \\ 0 & v_2 & 0 \\ a \cos \beta & \cos \alpha & c \end{vmatrix}$$

<sup>3</sup> Bond, W. L., *Am. Mineral.*, **31**, 31-42 (1946).

The columns contain the  $x$ ,  $y$ , and  $z$  components of the  $a$ ,  $b$ , and  $c$  axes respectively,  $v_1$  and  $v_2$  are the constants already given by equations 1-4 of Table 1. The transposed reciprocal of this matrix is also given by Bond:

$$\overline{M}^{-1} = \begin{vmatrix} \frac{1}{a \sin \beta} & 0 & -\frac{\cot \beta}{c} \\ -\frac{v_1}{av_2 \sin \beta} & \frac{1}{v_2} & \frac{v_1 \cot \beta - \cos \alpha}{v_2 c} \\ 0 & 0 & \frac{1}{c} \end{vmatrix}$$

Here the columns contain the Cartesian components of the axes of the reciprocal cell. The reciprocal axes have the ratio  $p_0:q_0:r_0 (= 1)$  and are separated by the interaxial angles  $\lambda$ ,  $\mu$  and  $\nu$ . By matrix multiplication of the reciprocal vectors (face normals) (001), (101), and (011) with  $\overline{M}^{-1}$ , their respective Cartesian components are obtained. If these vectors are extended to the gnomonic projection plane ( $z=1$ ), these components are then simple functions of the projection elements. The polar elements are then simply scaled down from the projection elements by the length of the (001) vector ( $r_0'$ ).

#### SUMMARY

Relationships have been derived among the three sets of triclinic elements, axial, projection and polar elements. These are given in a table as a list of formulae. They are derived by a study of vectors in the reciprocal cell and their components on Cartesian axes. It is hoped that they will be of use in triclinic calculations in general; for example: (1) to derive projection elements from references where only axial elements are given, for the purpose of making graphical measurements and crystal drawings; (2) to derive axial elements from projection elements obtained from newly measured crystals, as a check against published data, or for the preparation of new data; (3) to derive polar elements as a check against  $x$ -ray data.