THE DETERMINATION OF THE CRYSTALLOGRAPHIC CONSTANTS IN THE TRICLINIC SYSTEM

A. L. Parsons, *University of Toronto.*

The greatest pleasure that can be obtained from the measurement of a simple crystal and the calculation of its constants is in connection with a triclinic crystal. The system has been much abused and wrongfully so. When the calculation is made in connection with a gnomonic projection it becomes a very simple problem in solid trigonometry which offers absolutely no difficulty to a student who understands the rudiments of plane trigonometry. It is true that there are spherical triangles involved; in fact there are polar spherical triangles. The only characteristic about polar triangles that one needs to know is that the angles of one polar triangle are equal to 180° minus the opposite sides of the other polar triangle. When one of these triangles is solved the other is automatically solved. When the writer started the present paper it was his intention to give a graphic solution of the constants following the classical paper of Borgström and Goldschmidt,[1] which served as the model of his own paper on the same subject.[2] In proceeding with the work it became evident that a modification of the calculation offered many advantages in relating all the constants directly to two circle measurements so that the purpose of the present paper is to demonstrate a simple method of calculating the angular and linear constants of a triclinic crystal from measurements on the two circle goniometer.

For the calculation the forms (100), (010), (001), (011), ($\bar{1}$01), and ($\bar{1}$11) of copper sulphate ($CuSO_4 \cdot 5H_2O$) are employed, using the ϕ and ρ values given in Goldschmidt's Winkeltabellen and using the orientation adopted there.

The determination of the following constants is given graphically and mathematically:

Table I.

α	$\sin(\nu-\phi_0)\cdot\tan\rho_0=\cot\alpha$	av.
β	$\sin\phi_0\cdot\tan\rho_0=\cot\beta$	av.
γ	$\left\{\begin{array}{l}\cot\rho_0\cdot\cot\lambda=\sin\theta\\ \cot\rho_0\cdot\cot\mu=\sin\kappa\\ \theta+\kappa=\gamma\end{array}\right\}$	
λ	$\cos\phi_0\cdot\sin\rho_0=\cos\lambda$	av. of y_0'

[1] *Zeit. Kryst.*, **1906,** 41, 163.

[2] *Am. Mineral.*, **5,** pp. 190–194, 198–207.

μ	$\cos(\nu-\phi_0)\cdot\sin\rho_0=\cos\mu$	av. of w_0'
ν	measured direct	av.
	$a=\dfrac{\{[\sin(\nu-\phi)\cdot\tan\rho^{011}]-[\sin(\nu-\phi)\tan\rho^{001}]\}\sin\alpha}{[(\sin\phi\cdot\tan\rho\ \bar{1}01)-(\sin\phi\tan\rho^{001})]\sin\beta}$	av.
	$b=1$	
	$c=[\sin(\nu-\phi)\tan\rho^{011}]-[\sin(\nu-\phi^{001})\cdot\tan\phi^{001}]\sin\alpha$	av.
ϕ_0	measured direct ($=\phi$ for 001)	av.
ρ_0	measured direct ($=\rho$ for 001)	av.
	$p_0=p_0'\cos\rho_0$ (Gdt)	av.
	$q_0=q_0'\cos\rho_0$ (Gdt)	av.
$x_0'=$	$\sin\phi_0\tan\rho_0$	av.
$y_0'=$	$\cos\phi_0\tan\rho_0$	
$w_0'=$	$\sin(\nu-\phi_0)\tan\rho_0$	av.
$u_0=$	$\cos(\nu-\phi_0)\tan\rho_0$	

The arithmetical calculation has been made in each case and yielded a perfect check for the angles and a maximum variation of three in the fourth decimal place for a and c, so that only the formulae employed are given.

In the graphical determination of the angles the angle point has been determined for the plane in which the angle lies in all cases. Where this angle point comes on the ground circle, in general no special mention is made of the fact inasmuch as the angle point for any plane passing through the pole lies on the ground circle.

Determination of α.

From the projection (fig. 1) it is evident that

$$\sin(\nu-\phi_0)\cdot\tan\rho_0=\cot\alpha=\cot(180^0-\alpha)$$

for

$$\sin(\nu-\phi_0)=\frac{OA}{OF}$$

and

$$\tan\rho_0=\frac{OF}{1}\cdot$$

The average value of α may be obtained from all terminal faces as follows:

$$\sin(\nu-\phi)\cdot\tan\rho=\cot T=w'+qq_0'\cdot\sin\nu$$

and

$$\frac{w'}{1}=\cot\alpha.$$

Determination of $c{:}b$ (fig. 1), for forms (011), (111), ($\bar{1}$11), (211), etc.

$$\sin\nu-\phi\cdot\tan\rho=\cot\xi$$

$$(\cot\xi-\cot\alpha)\cdot\sin\alpha=\frac{c}{b}$$

$$b=1$$

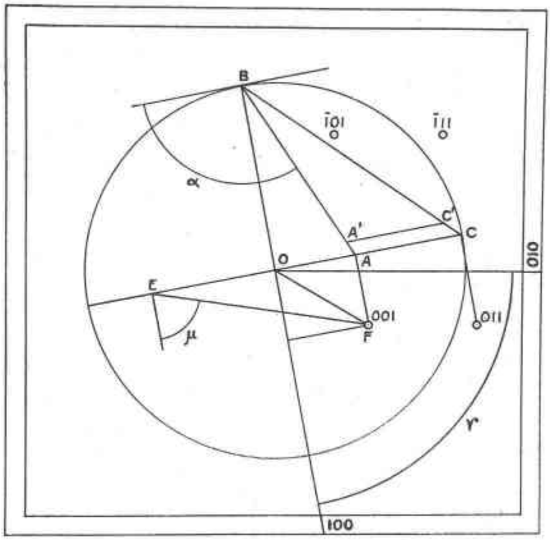

Figure 1.

Determination of μ (fig. 1).

From the projection it is also evident that

$$\cos(\nu-\phi_0)\cdot\sin\rho_0=\cos\mu$$

Graphic Determination of μ.

Locate E the angle point of the zone 001–101. Then μ is the angle between 001 and 100.

Determination of ν (fig. 1).

For the determination of ν we have the direct measurement of the angle between the normals to the faces (100) and (010).

An average value of ν may be obtained from the rectangular co-ordinates of pairs of faces in the same zones as (010) and (100), respectively.

In the first case:

$$\frac{x_1-x_2}{y_1-y_2}=\tan 0°$$

In the second case:

$$\frac{x_1-x_2}{y_1-y_2}=\tan\nu$$

If instead of tan 0° we have a positive or negative value the corresponding angle must be subtracted from or added to the value of ν which is obtained from the second calculation.

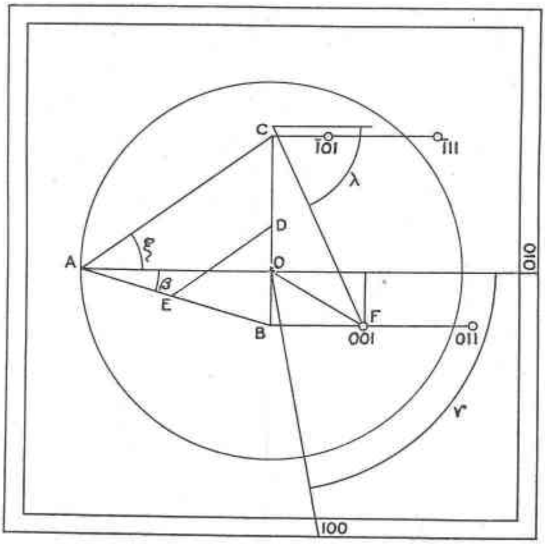

Figure 2.

Determination of β.

From the projection (fig. 2) it is evident that

$$\sin \phi_0 \cdot \tan \rho_0 = \cot \beta = \cot 180^0 - \beta$$

for $$\sin \phi_0 = \frac{BO}{OF}$$

and $$\tan \rho_0 = \frac{OF}{1} = \frac{x_0'}{1} \cdot$$

The average value for β may be obtained from all terminal faces as follows:

$$\sin \phi \cdot \tan \rho = \cot \Sigma = x_0' + pp_0' \cdot \sin \nu$$

and $$\frac{x_0'}{1} = \cot \beta$$

Determination of λ (fig. 2).

It is also evident from the same figure that

$$\cos \phi_0 \cdot \sin \rho_0 = \cos \lambda = \cos(180^0 - \lambda)$$

The average value of λ is obtained from the average value of y_0'.

Determination of c:a and a:b (fig. 2).

For the forms in the zone $(\bar{1}01)$ and $(\bar{1}11)$

$$\sin \phi \cdot \tan \rho = \cot \xi$$

$$\cot \xi - \cot \beta = \frac{CB}{OA}$$

$$\frac{CB}{OA} \cdot \sin\beta = \frac{CB}{AB} = \frac{c'}{a'} = \frac{c}{a} \cdot$$

Taking $DB=C$ (determined in fig. 1) and drawing $DE \| AC$

then
$$\frac{DB}{EB}=\frac{c}{a}$$

and
$$EB=a.$$

By calculation
$$\frac{\frac{c}{b}}{\frac{c}{a}}=\frac{a}{b}=\frac{a}{1}=a.$$

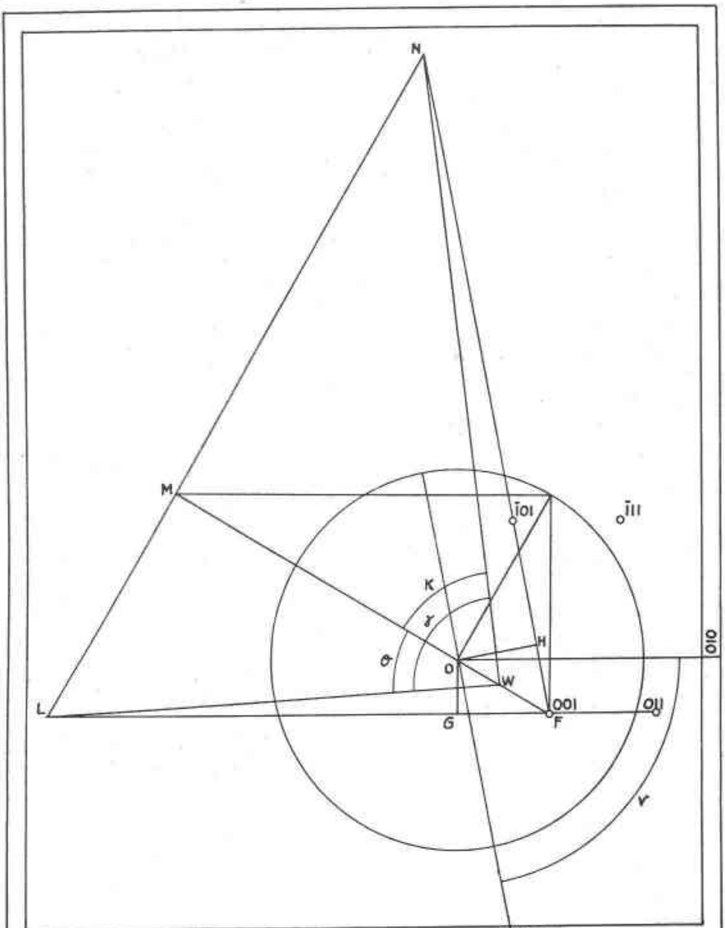

Figure 3.

Determination of γ (fig. 3).

In the plane of 001 we take the angles between the traces of the zone 001–010 and of the plane of the pole and $001 = \theta$, and between the zone 001–100 and of the plane of the pole and $001 = \kappa$, then

$$\cot \rho_0 \cot \lambda = \sin \theta$$

and

$$\cot \rho_0 \cdot \cot \mu = \sin \kappa$$

and

$$\theta + \kappa = \gamma$$

Graphical determination of γ.

Locate M at 90° from F (001). Draw LN perpendicular to FM intersecting FN and FL at N and L. Determine the angle point W. Then $\angle NWL = \gamma$.

Determination of ϕ_0, $\nu - \phi_0$, *and* ρ_0.

In a former paper[3] the equations are given that are necessary for obtaining the best average values for x_0', y_0', ρ_0 and ϕ_0. From the average values of ϕ_0 and ν we obtain a good average of $(\nu - \phi_0)$.

Conclusion

The formulae that are given above furnish a simple means of determining the constants of a triclinic crystal with a high degree of accuracy. More good average values can be obtained than by previous methods. The readings on the goniometer are accurate only to the nearest minute. By using average values the constants in most cases can be obtained in seconds. The accuracy of the ratio $a:b:c$ depends upon accuracy of angles to seconds. With α, β and γ determined to the nearest minute there is an error in the fourth decimal place in the ratio $a:b:c$.

By the graphical methods shown a high degree of accuracy can be obtained both for the angular and linear constants.

The most important feature of the method lies in the fact that the results of two circle measurements of crystals can be compared with the constants that have been obtained by other methods without tedious calculation. In general the accuracy of the graphical solution is sufficient.

The methods shown here for the general case are readily employed for the special cases of the other crystal systems.

[3] *Am. Mineral.*, **5**, pp. 204, 205 and 207.