

## APPROXIMATE FORMULAE FOR TRICLINIC CALCULATIONS\*

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### ABSTRACT

Approximation formulae are presented which allow the calculation of the elements of a triclinic lattice from those of the corresponding reciprocal lattice and vice-versa. These formulae, which do not require the use of trigonometric tables, are highly accurate for lattice angles close to 90°. Their value for approximate calculations when the angles depart from 90° is also discussed in the paper.

The usual formulae for the calculation of the elements of the triclinic system (cf. Buerger 1942, Chap. 18) are cumbersome and require many references to trigonometric tables. Various graphical and nomographic methods have been suggested (e.g. Bond 1950) but all these require special facilities. The present note presents a type of approximation formula which is surprisingly accurate, is well adapted to machine or slide rule calculation, and avoids the use of trigonometric tables.

Consider first the formula

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

which with its inversion and with cyclic permutations permits the calculation of the crystal lattice angles  $\alpha$ ,  $\beta$ ,  $\gamma$  from the reciprocal lattice angles  $\alpha^*$ ,  $\beta^*$ ,  $\gamma^*$  and vice versa. Adopting the notation

$$\bar{\alpha} = \pi/2 - \alpha \text{ (etc.)}, \quad (2)$$

we may write (1), in terms of the complements of the angles, as

$$\sin \bar{\alpha} = \frac{\sin \bar{\beta}^* \sin \bar{\gamma}^* - \sin \bar{\alpha}^*}{\cos \bar{\beta}^* \cos \bar{\gamma}^*}. \quad (3)$$

Using standard methods, discussed briefly below, this expression may be expanded in series in the form

$$\bar{\alpha} \approx -\bar{\alpha}^* + \bar{\beta}^* \bar{\gamma}^* - \frac{1}{2} \bar{\alpha}^* (\bar{\beta}^{*2} + \bar{\gamma}^{*2}) \quad (4)$$

where the angles are expressed in radians. If the angles are expressed in degrees, (4) must be written

$$\begin{aligned} \bar{\alpha} &\approx -\bar{\alpha}^* + K \bar{\beta}^* \bar{\gamma}^* - \frac{1}{2} K^2 \bar{\alpha}^* (\bar{\beta}^{*2} + \bar{\gamma}^{*2}) \\ &= -T_1 + K T_2 - K^2 T_3. \end{aligned} \quad (5)$$

The two fourth degree terms omitted from the expansion (5) are

$$K^3 (T_4 + T_4') = \frac{1}{2} K^3 \bar{\alpha}^{*2} \bar{\beta}^* \bar{\gamma}^* + \frac{1}{3} K^3 \bar{\beta}^* \bar{\gamma}^* (\bar{\beta}^{*2} + \bar{\gamma}^{*2}). \quad (5')$$

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In these expressions, the symbols  $T_1, T_2$ , etc., are introduced to simplify the later discussion, and the constant  $K = \pi/180^\circ$  and its powers have the values:

$$\begin{array}{ll} K = 1.7453 \times 10^{-2} & K^{-1} = 5.7296 \times 10 \\ K^2 = 3.0462 \times 10^{-4} & K^{-2} = 3.2828 \times 10^3 \\ K^3 = 5.3166 \times 10^{-6} & K^{-3} = 1.8809 \times 10^5 \\ K^4 = 9.2792 \times 10^{-8} & K^{-4} = 1.0777 \times 10^7 \end{array}$$

In Table 1, the errors ( $\epsilon$ ) for the expansion (5) and its abbreviated forms are calculated for the several ranges  $\epsilon = 0.5^\circ, 0.05^\circ, 0.005^\circ$  which correspond to calculations which may be taken as valid respectively to

TABLE 1. ERROR ANALYSIS FOR EQUATION (5)  
Angles expressed in degrees

Approximation formula	Term omitted	Permitted Error $\epsilon$		
		$\epsilon < 0.5^\circ$	$\epsilon < 0.05^\circ$	$\epsilon < 0.005^\circ$
(5a) $\bar{\alpha} = -\bar{\alpha}^*$	$T_2$	$< 28.6$	$< 2.86$	$< 0.286$
	AR	$< 5.35^\circ$	$< 1.69^\circ$	$< 0.54^\circ$
(5b) $\bar{\alpha} = -\bar{\alpha}^* + K\bar{\beta}^*\bar{\gamma}^*$	$T_3$	$< 1.64 \times 10^3$	$< 1.64 \times 10^2$	$< 1.64 \times 10$
	AR	$< 11.8^\circ$	$< 5.47^\circ$	$< 2.54^\circ$
(5) $\bar{\alpha} = -\bar{\alpha}^* + K\bar{\beta}^*\bar{\gamma}^*$ $-\frac{1}{2}K^2\bar{\alpha}^*(\bar{\beta}^{*2} + \bar{\gamma}^{*2})$	$T_4$	$< 9.40 \times 10^4$	$< 9.40 \times 10^3$	$< 9.40 \times 10^2$
	AR	$< 20.8^\circ$	$< 11.7^\circ$	$< 6.59^\circ$
	$T_4'$	$< 9.40 \times 10^2$	$< 9.40 \times 10^3$	$< 9.40 \times 10^2$
	AR	$< 19.4^\circ$	$< 10.9^\circ$	$< 6.13^\circ$

$1^\circ, 0.1^\circ, 0.01^\circ$ . Under each formula and each value of  $\epsilon$  the useful range is expressed in two ways: in the upper line as the maximum range for the leading term ( $T_2, T_3$ , etc.) omitted, and in the lower line in terms of the angle range (AR) permitted in the most unfavorable case in which all the angles involved in the omitted term have the same value. The error ranges chosen for calculation in Table 1 are based on the errors met with in the usual goniometric and x-ray analytic techniques. Most work should be better than  $\epsilon = 0.05^\circ$  which corresponds to a value accurate to  $0.1^\circ$ , while it is only exceptional work which reaches  $\epsilon = 0.005^\circ$  accurate to  $0.01^\circ$ .

From Table 1, it is clear that the simplest formula

$$\bar{\alpha} = -\bar{\alpha}^* \tag{5a}$$

is of value only for the roughest calculations. It will however give a

determination of the correct sign<sup>1</sup> for  $\bar{\alpha}$  in all cases in which  $\bar{\alpha}^*$  and  $\bar{\beta}^*\bar{\gamma}^*$  have opposite sign, and in those cases of the same sign in which  $|\bar{\beta}^*\bar{\gamma}^*| > 57.3|\bar{\alpha}^*|$ , i.e. (5a) will then give the incorrect sign when  $\bar{\alpha}^*$  is very small compared with  $\bar{\beta}^*$  and  $\bar{\gamma}^*$ . The second approximation given by the formula

$$\bar{\alpha} = -\bar{\alpha}^* + K\bar{\beta}^*\bar{\gamma}^* \quad (5b)$$

is adequate for almost all crystallographic work for angles up to  $3^\circ$  or  $4^\circ$  and for rough calculations it can be used up to  $6^\circ$ . The third approximation of (5) will enable the calculations to be carried out to  $0.01^\circ$  for angles up to  $6^\circ$  and will be satisfactory for many calculations up to  $10^\circ$  or  $12^\circ$ . It is of course possible to add the fourth degree terms of equation (5') to those of (5) if higher precision is desired over a wider range of angle, but under such circumstances it is undoubtedly better to have recourse to the original expression (1) and the trigonometric tables.

If we solve equation (1) for  $\cos \alpha^*$  we obtain the expression

$$\cos \alpha^* = \cos \beta^* \cos \gamma^* - \sin \beta^* \sin \gamma^* \cos \alpha, \quad (6)$$

which is used in those cases in which one crystal angle and two reciprocal angles are measured (e.g. on the Buerger precession camera when two zero layers at a known angle apart have been photographed). Equation (6) can be expanded in the form

$$\bar{\alpha}^* = -\bar{\alpha} + K\bar{\beta}^*\bar{\gamma}^* + \frac{1}{2}K^2\bar{\alpha}(\bar{\beta}^{*2} + \bar{\gamma}^{*2}). \quad (7)$$

Since the terms of this expression differ only in detail from those of (5), the error discussion of Table 1 is directly applicable here.

The expanded form of the expression for the volume of the cell is particularly convenient and quite accurate. The usual expression

$$V = V_0[1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma]^{1/2} \quad (8)$$

becomes

$$V = V_0[1 - \frac{1}{2}K^2(\bar{\alpha}^2 + \bar{\beta}^2 + \bar{\gamma}^2) + K^3\bar{\alpha}\bar{\beta}\bar{\gamma}], \quad (9)$$

in which  $V_0 = abc$ . The largest term omitted is

$$K^4T_4 = (K^4/24)[(\bar{\alpha}^4 + \bar{\beta}^4 + \bar{\gamma}^4) - 6(\bar{\beta}^2\bar{\gamma}^2 + \bar{\gamma}^2\bar{\alpha}^2 + \bar{\alpha}^2\bar{\beta}^2)]. \quad (9')$$

The error analysis for (9) is given in Table 2. From it we see that the simplest result  $V = V_0$  is sufficiently accurate for the determination of the number of molecules per cell even for quite large angles. The complete expression (9) which is quite simple to use is adequate for almost all

<sup>1</sup> Difficulty cannot arise from the term  $T_3$  since it always has the sign of  $T_1$ . The terms  $T_4$  and  $T_4'$  cannot enter unless the complementary reciprocal lattice angles reach the extraordinary values of  $70-80^\circ$ .

TABLE 2. ERROR ANALYSIS FOR EQUATION (9)  
Angles expressed in degrees

Approximation formula	Term omitted	Permitted Error $\epsilon$		
		$\epsilon < 5\%$	$\epsilon < 0.5\%$	$\epsilon < 0.05\%$
(9a) $V = V_0$	$T_2$ AR	$< 161$ $< 10.5^\circ$	$< 16.1$ $< 3.31^\circ$	$< 1.61$ $< 1.05^\circ$
(9b) $V = V_0[1 - \frac{1}{2}K^2(\bar{\alpha}^2 + \bar{\beta}^2 + \bar{\gamma}^2)]$	$T_3$ AR	$< 9.40 \times 10^3$ $< 21.1^\circ$	$< 9.40 \times 10^2$ $< 9.80^\circ$	$< 9.40 \times 10$ $< 4.55^\circ$
(9) $V = V_0[1 - \frac{1}{2}K^2(\bar{\alpha}^2 + \bar{\beta}^2 + \bar{\gamma}^2) + K^3\bar{\alpha}\bar{\beta}\bar{\gamma}]$	$T_4$ AR	$< 5.39 \times 10^5$ $< 30.5^\circ$	$< 5.39 \times 10^4$ $< 17.1^\circ$	$< 5.39 \times 10^3$ $< 9.64^\circ$

structure analytical calculations provided the cell angles are within  $10^\circ$  of right angles.

It is perhaps worth while to outline briefly the steps involved in one of these expansions. Equation (3) may be rewritten in the form

$$\sin \bar{\alpha} = \tan \bar{\beta}^* \tan \bar{\gamma}^* - \sec \bar{\beta}^* \sec \bar{\gamma}^* \sin \bar{\alpha}^*.$$

The power series for the trigonometric functions (see, for example, Pierce 1929, pp. 91-92) permit the expansion

$$\begin{aligned} \sin \bar{\alpha} = & (\bar{\beta}^* + \bar{\beta}^{*3}/3)(\bar{\gamma}^* + \bar{\gamma}^{*3}/3) \\ & - (1 + \bar{\beta}^{*2}/2 + 5\bar{\beta}^{*4}/24)(1 + \bar{\gamma}^{*2}/2 + 5\bar{\gamma}^{*4}/24)(\bar{\alpha}^* - \bar{\alpha}^{*3}/6) \end{aligned}$$

in which terms higher than the fourth power in the angles are omitted. Carrying out the multiplication we get

$$\sin \bar{\alpha} = -\bar{\alpha}^* + \bar{\beta}^*\bar{\gamma}^* - \frac{1}{2}\bar{\alpha}^*(\bar{\beta}^{*2} + \bar{\gamma}^{*2}) + \bar{\alpha}^{*3}/6 - \frac{1}{2}\bar{\alpha}^*(\bar{\beta}^{*2} + \bar{\gamma}^{*2}).$$

We now invert the usual series for  $\sin \bar{\alpha}$  in the form

$$\bar{\alpha} = \sin \bar{\alpha} + (\sin^3 \bar{\alpha})/6$$

and obtain

$$\bar{\alpha} = -\bar{\alpha}^* + \bar{\beta}^*\bar{\gamma}^* - \frac{1}{2}\bar{\alpha}^*(\bar{\beta}^{*2} + \bar{\gamma}^{*2}) + \frac{1}{2}\bar{\alpha}^{*2}\bar{\beta}^*\bar{\gamma}^* + \frac{1}{3}\bar{\beta}^*\bar{\gamma}^*(\bar{\beta}^{*2} + \bar{\gamma}^{*2}).$$

Similar techniques can be applied to the expansion of (6) and (8) and to the discussion of similar expansions of other formulae which may interest the reader.

#### REFERENCES

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