

Table 1. *Crystallographic data*

Compound	Evolidine		
	Valinomycin	Iodoacetate	(Transf. prod.)
Formula	$C_{36}H_{60}O_{12}N_4$	$C_{40}H_{59}O_{10}N_8I$?
Unit cell dimensions			
<i>a</i>	10.4 ₄ (Å)	9.35 Å	9.23 Å
<i>b</i>	14.47	22.5	23.0
<i>c</i>	22.2 ₂	24.9	25.3
α°	105.0°	—	—
β°	86.9°	—	—
γ°	90.4°	—	—
Space group	P1	$P2_12_12_1$	$P2_12_12_1$
Density (g.cm. ⁻³)			
Meas.	1.15	—	—
Calc.	1.13	1.15	—
Number of molecules	3	4	—

Acta Cryst. (1959). **12**, 479

A new aid for the rapid determination of absorption corrections by Albrecht's method.

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(Received 17 January 1959)

Albrecht's (1939) method for graphically determining the correction for absorption of the X-ray beam by a crystal is useful when the crystal cannot be ground into a sphere or cylinder and when automatic computing machinery is not available. Recently Rogers & Moffett (1956) and Henshaw (1958) have published aids to facilitate the procedure. The following modification of the methods already described is an added timesaver.

Albrecht approximated the absorption correction for a crystal of constant cross-section by the expression

$$A = N^{-1} \sum_{j=1}^N \exp \{-\mu(l_i + l_r)_j\},$$

where μ is the linear absorption coefficient, l_i and l_r are respectively the lengths of the j th incident and diffracted rays, and N is the total number of regularly-spaced points in the cross-section, at which

$$\exp \{-\mu(l_i + l_r)_j\}$$

was evaluated.

In previous methods l_i and l_r were determined in separate operations. It is possible, however, to measure

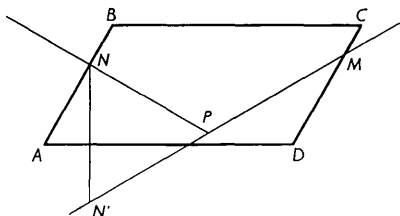


Fig. 1. The path of X-rays reflected at a single point in a crystal. $ABCD$ is the outline of a crystal, NP is the incident ray, and PM is the diffracted ray.

I am extremely grateful to Dr L. C. Vining of the Prairie Regional Laboratory, National Research Council, Saskatoon, Saskatchewan, Canada for the preparation and gift of beautiful crystals of valinomycin, to Prof. A. J. Birch, of the University of Manchester, U. K. for his kindness in presenting a quantity of the rare natural product, evolidine, and to Mr A. F. Beecham of this Division for preparing the iodoacetate derivative of evolidine.

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($l_i + l_r$) directly and evaluate each term of the summation in a single step. In Fig. 1, a ray enters the crystal at N , is reflected at P , and emerges at M . If a point N' on the extension of PM can be located such that NP is equal in length to $N'P$, the length NN' must represent ($l_i + l_r$). Because the triangle NPN' is isosceles, the line NN' makes equal angles with NP and $N'P$, and this angle is the complement of the Bragg angle. The line through NN' , therefore, must be parallel to the reciprocal lattice vector for the reflection under consideration and is the same for all diffracted rays originating on the same incident ray. By measuring NN' with an exponential scale, one obtains a term of the summation for each chosen point P .

The measurement is made with the aid of one drawing and four overlays. The lowermost sheet (as suggested by Rogers & Moffett, 1956) has a plot of the reciprocal lattice and a correctly oriented outline of the crystal on the scale $\alpha = m\mu x$, where x is the actual dimension, α the corresponding distance in the outline, and m a constant dependent on the exponential scale on which the path lengths within the crystal are measured. Sheets two and three are Bernal circles for the incident and diffracted ray, on the same scale as the reciprocal lattice. Both of these sheets have equally spaced parallel lines for establishing the network of points at which the absorption correction will be evaluated, as described by Rogers & Moffett (1956). Sheets four and five carry the exponential scales for reading the individual absorption terms.

The two scales are mounted on rectangular sheets of clear celluloid. Each sheet must have one straight edge and an inscribed line parallel to it, both lines being the same distance (e.g. 2.5 cm.) from the edge. The scale for l_i , termed the entrance scale, is made by marking a zero point, Z , near one end of a narrow strip of paper. The exit scale, on which ($l_i + l_r$) is actually measured, is

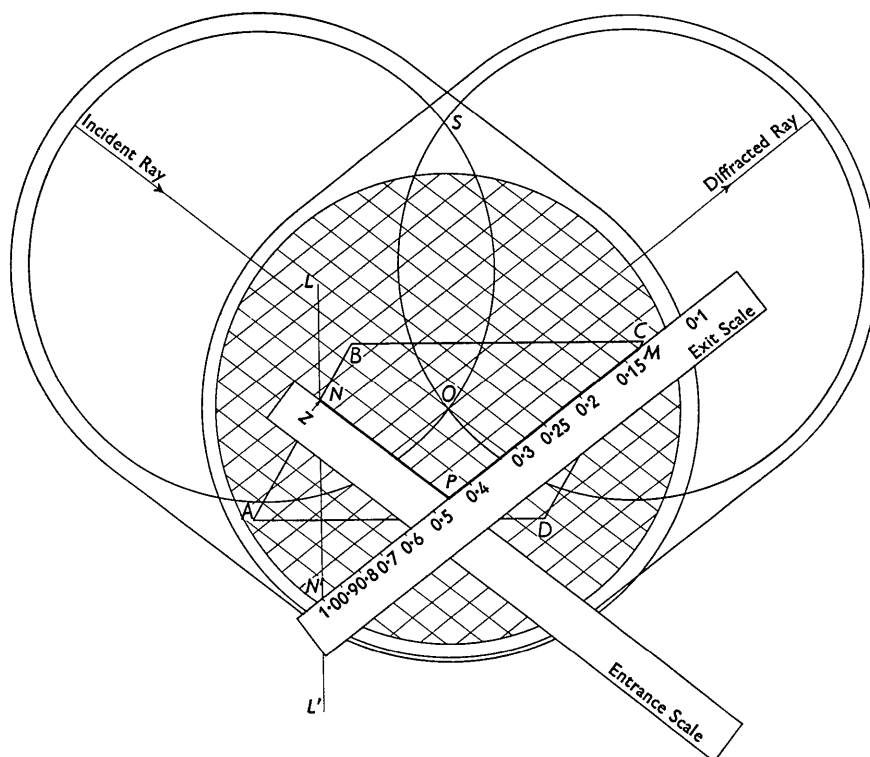


Fig. 2. Position of the scales for reading one absorption term in the summation. Point S is the reciprocal lattice point under consideration, and LL' is the inscribed line. The reciprocal lattice drawing has been omitted for clarity. The remaining symbols are identified in Fig. 1.

constructed by marking appropriate values of $\exp(-\alpha/m)$ at corresponding distances $\alpha = m\mu x$ on a similar strip of paper. This exponential scale can be quickly traced from the C scale of a 10-inch slide rule ($m = 11.03$) or a 25-centimeter slide rule ($m = 10.86$).

The scales are set with the aid of a drafting machine with the Bernal circles or other device that maintains a movable straight edge at a fixed orientation as shown in Fig. 2. Adjust the drafting machine so that one arm is parallel to the desired reciprocal lattice vector OS . Place one sheet of celluloid with its straight edge against the arm of the drafting machine. Attach the entrance scale, parallel to the incident beam, so that its zero point, Z , is on the inscribed line. Place the second sheet of celluloid against the arm like the first and attach the exit scale parallel to the diffracted beam, with its zero point ($\alpha = 0$) on the inscribed line.

To read the correction terms, move the drafting machine so that the entrance scale lies along one of the parallel lines representing incident rays, with its zero at the entry point N . Keeping the exit scale sheet against

the drafting machine and sliding it to the position where this scale intersects the entrance scale at point P , read $\exp(-\mu x)$ for point P at M . Repeat this operation for all points on the network within the crystal outline, summing the terms on a desk calculator which also accumulates the number of terms. Divide the two final figures to obtain the desired value for the absorption correction.

The entrance scale actually can be eliminated, but the author believes its presence will reduce the chance of skipping a point or reading one twice. Like Rogers & Moffett (1956), the author has found that sufficiently accurate values can be obtained by determining A for only a few lattice points and interpolating the rest.

References

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