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## Setting a single crystal by non-equatorial X-ray reflexions.

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Normal X-ray methods of orienting a crystal to rotate accurately about a principal symmetry axis fail when no reflexions in the equatorial layer line can be identified. A review of methods hitherto published is included in a comprehensive paper by Jeffery (1949) but to meet a particular problem, not covered by methods discussed by Jeffery, a technique was developed which has a wider applicability.

It was necessary to set a crystal of a lamellar mineral to rotate accurately about the sixfold axis perpendicular to the lamellae. From the external form this could easily be done to within 5°, but as the hexagonal unit cell had dimensions $a = 9{\cdot}7$ and $c = 133$ Å it was quite impossible to identify equatorial reflexions. As the row lines were well separated the following method was used.

Three 5°-oscillation photographs were taken on the same film at exactly 120° intervals of azimuth (using a Unicam single-crystal X-ray goniometer). To enable these three superimposed photographs to be distinguished, the cassette was rotated by about 2° to each side of its normal position so that the three equivalent row lines appeared side by side. When exactly set to rotate about the hexad axis, corresponding features on the three row lines lie at the same distance from the equator of the photograph, but when mis-set their relative displacements give the corrections necessary.

Suppose $\alpha_1$, $\alpha_2$ and $\alpha_3$ were the angular distances of three equivalent reciprocal-lattice vectors from the axis of rotation. The distances $y_1, y_2$ and $y_3$ of the corresponding reflexions from an equatorial line scribed on the film were measured as accurately as possible and $\zeta_1$, $\zeta_2$ and $\zeta_3$ were obtained from $\zeta = y(r^2+y^2)^{-\frac{1}{2}}$. $\xi$ for the particular row line used was calculated or measured and hence, from $\cot\alpha = \zeta/\xi$, $\alpha_1$, $\alpha_2$ and $\alpha_3$ were found. As the differences of $\alpha$ values are small (less than 5°), and as infinitesimal rotations can be treated as vectors, the resultant of three vectors of magnitudes $(90°-\alpha_1)$, $(90°-\alpha_2)$ and $(90°-\alpha_3)$ spaced 120° apart gave the magnitude and direction of the necessary correction. The direction of this correction was known to $\pm 2\frac{1}{2}°$ from the oscillation range. The angular correction was resolved into two components parallel to the two arcs. Adding the vectors, relating them to the positions of the arcs, and resolving the resultant correction parallel to the arcs were done graphically. If the initial setting of the lower arc were far from zero, correction for the tilt of the upper arc would have to be applied, being found by solving a spherical triangle. The corrections obtained are not exact and two applications are necessary for setting to 0·1°.

The method can of course be used for other than sixfold axes if the rotation intervals are chosen appropriately.

### Reference

Jeffery, J. W. (1949). *Acta Cryst.* **2**, 15.

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## The direct-inspection method in systems with a principal axis of symmetry.

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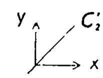
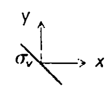
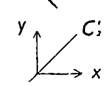
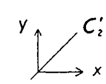
The direct-inspection method (Fumi, 1952*a*)* can be used *to obtain directly* the independent components of tensor properties of matter only for symmetry groups in which one can find Cartesian orthogonal coordinates that do not transform into linear combinations of themselves under the independent symmetry elements. The Cartesian orthogonal reference frames usually applied for groups with a principal axis $C_n (n \geq 3)$ ($z||$to the axis, $x$ and $y \perp$ to it) satisfy this condition only for $n = 4$, but there are other frames which allow direct inspection in

Table 1

| Finite groups with a principal axis $C_n (n \geq 3)$ | | Generating elements besides $C_n$ | Possible choices of $x$ and $y$ | | |
|---|---|---|---|---|---|
| $n$ even | $n$ odd | | | | |
| $D_n$ | $D_n$ | $C_2'$ | $x\|\|C_2'$ | $y\|\|C_2'$ |  |
| $C_{nv}$ | $C_{nv}$ | $\sigma_v$ | $yz\|\|\sigma_v$ | $zx\|\|\sigma_v$ |  |
| $C_{nh}$ | $C_{nh}$ | $\sigma_h$ | | Any | |
| $D_{nh}$ | $D_{nh}$ | $C_2'$, $\sigma_h$ | $x\|\|C_2'$ | $y\|\|C_2'$ |  |
| | $C_{ni}$ | $i$ | | Any | |
| | $D_{nd}$ | $C_2'$, $i$ | $x\|\|C_2'$ | $y\|\|C_2'$ |  |

$C_2'$ = binary axis $\perp C_n$; $\sigma_v(\sigma_h)$ = symmetry plane$||(\perp)C_n$; $i$ = inversion.

* In this paper § 3 (*a*) is somewhat too condensed to be completely clear. Equations (9) and (10), like equations (6) and (7), are relations between equations (3); when written fully, equation (9) reads

$$t_{xyz} = t_{yzx} = t_{zxy} = t_{xzy} = t_{yxz} = t_{zyx}.$$

The last sentence of § 3 (*a*) states the identity of the scheme of independent components of the axial and polar third-order tensors for symmetry $O$ with the scheme of the axial third-order tensor for symmetry $T_d$.