

Les directions principales font avec les axes des angles, exprimés en degrés, très voisins de

	a	b'	c'
$\chi_{11}$	$73,7 \pm 0,1$	$76,5 \pm 0,2$	$158,6 \pm 0,2$
$\chi_{22}$	$89,5 \pm 0,1$	$14,2 \pm 0,2$	$75,8 \pm 0,2$
$\chi_{33}$	$16,3 \pm 0,1$	$94,4 \pm 0,1$	$74,4 \pm 0,1$

Ces résultats sont nettement différents de ceux de Banerjee (1938) qui proposait  $\chi_1 = -0,093$ ,  $\chi_2 = -0,263$  et  $\chi_3 = -0,125 \text{ mm}^3 \text{ mol}^{-1}$  avec  $\chi_3$  suivant **b'**. Pour nous, l'axe  $\chi_{11}$  est dirigé suivant l'axe **M** des deux molécules qui correspond, dans la structure, à l'intersection des deux plans moléculaires. Les axes  $\chi_{22}$  et  $\chi_{33}$  correspondent respectivement aux résultantes des axes **L** des deux molécules d'une part et des axes **N** d'autre part. Ces résultats justifient la procédure adoptée pour déterminer les valeurs théoriques des angles, les susceptibilités cristallines principales et les susceptibilités moléculaires principales. Nous signalerons que l'utilisation des valeurs angulaires de Banerjee (1938) conduit à des résultats dénués de sens physique. Les anisotropies moléculaires déduites du tableau précédent sont largement indépendantes de la valeur adoptée pour la susceptibilité moyenne [ $\bar{\chi} = -0,1603$ ,  $-0,167$ ,  $-0,168$  ou  $-0,1735 \text{ mm}^3 \text{ mol}^{-1}$ , suivant Landolt-Börnstein (1967)]. Par ailleurs, elles sont cohérentes avec les valeurs calculées antérieurement pour les autres composés aromatiques condensés (Van den

Bossche & Sobry, 1981). Ainsi, l'anisotropie dans le plan est de l'ordre de trois fois celle que nous avons calculée pour le naphthalène, qui était comprise entre  $0,00114$  et  $0,0026 \text{ mm}^3 \text{ mol}^{-1}$ . De même, la valeur calculée de  $K_L - K_N$  à partir du modèle simplifié que nous avons décrit est donnée par  $4x + 4,88y + 3z = 0,2278 \text{ mm}^3 \text{ mol}^{-1}$ , en bon accord avec les deux dernières que l'on déduit du tableau précédent.

Les auteurs remercient M. le Professeur J. Toussaint pour l'intérêt manifesté et pour son aide logistique et financière. Ils expriment aussi leur reconnaissance à M. le Professeur A. Van de Vorst qui a partiellement subventionné ce travail.

### Références

- BANERJEE, S. (1938). *Z. Kristallogr.* **100**, 316–355.  
 CAMPBELL, R. B. & ROBERTSON, J. M. (1962). *Acta Cryst.* **15**, 289–290.  
 LANDOLT-BÖRNSTEIN (1967). Band II, Teil 10, *Magnetische Eigenschaften* II. Berlin: Springer.  
 ROBERTSON, J. M., SINCLAIR, V. C. & TROTTER, J. (1961). *Acta Cryst.* **14**, 697–704.  
 VAN DEN BOSSCHE, G. & SOBRY, R. (1981). *Acta Cryst.* **A37**, 211–219.

*Acta Cryst.* (1982). **A38**, 287–288

**Polarization factor for the X-ray powder diffraction method with a single-crystal monochromator.** BY  
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(Received 29 July 1981; accepted 3 November 1981)

### Abstract

The polarization correction for X-ray diffraction with a single-crystal monochromator was derived by Azaroff [*Acta Cryst.* (1955), **8**, 701–704]. The correction was restricted to the arrangement in which the monochromator is set before the specimen crystal. In this case, the incident X-ray beam is monochromatized first, then projected on the specimen crystal. The inverse arrangement in which the monochromator is set after the specimen crystal is often used in powder diffraction. In this case, the X-ray beam is diffracted by the specimen crystal first, then monochromatized. This paper is an attempt to derive the polarization factor for the latter arrangement of the specimen crystal and the monochromator.

### Polarization factor

For simplicity, the same setting and the symbols are used as by Azaroff (1955), except that the plane  $P_1$  by which the X-ray is diffracted first, is the specimen crystal plane, and

the plane  $P_2$  by which the X-ray is secondly diffracted, is the single-crystal plane of the monochromator. The equations quoted from Azaroff are expressed by the same numbers as in his paper with the prefix 'A'.

From equations (A3) and (A7), the intensity of the first diffracted X-ray beam is expressed as

$$I' = \frac{1}{2}k^2 I_0 (1 + \cos^2 2\theta_1). \quad (1)$$

From equation (A13), the intensity of the second diffracted X-ray beam is expressed as

$$I'' = \frac{1}{2}k^2 k'^2 I_0 [(\cos^2 2\theta_1 \cos^2 \rho + \sin^2 \rho) \cos^2 2\theta_2 + \cos^2 2\theta_1 \sin^2 \rho + \cos^2 \rho]. \quad (2)$$

When the monochromator is set before the specimen crystal, the final intensity is expressed from (1) and (2) as

$$I''/I' = k'^2 [(\cos^2 2\theta_1 \cos^2 \rho + \sin^2 \rho) \cos^2 2\theta_2 + \cos^2 2\theta_1 \sin^2 \rho + \cos^2 \rho] (1 + \cos^2 2\theta_1)^{-1}, \quad (3)$$

which is the same as equation (A14).

When the monochromator is set after the specimen, the final intensity can be expressed in terms of the incident X-ray intensity. From (2), the ratio is obtained as

$$I''/I_o = \frac{1}{2}k^2 k'^2 [(\cos^2 2\theta_1 \cos^2 \rho + \sin^2 \rho) \cos^2 2\theta_2 + \cos^2 2\theta_1 \sin^2 \rho + \cos^2 \rho]. \quad (4)$$

Then the polarization factor  $P$  is expressed as

$$P = \frac{1}{2}[(\cos^2 2\theta_1 \cos^2 \rho + \sin^2 \rho) \cos^2 2\theta_2 + \cos^2 2\theta_1 \sin^2 \rho + \cos^2 \rho]. \quad (5)$$

For the powder method in which the specimen rotation axis is parallel to the diffraction plane of the monochromator crystal,  $\rho$  is fixed at zero. Then the polarization factor is reduced to

$$P = \frac{1}{2}(1 + \cos^2 2\theta_1 \cos^2 2\theta_2), \quad (6)$$

where  $\theta_1$  is the diffraction angle of the specimen crystal, and  $\theta_2$  is the diffraction angle of the monochromator crystal.

When the monochromator is set before the specimen crystal, (3), *i.e.* equation (A14) or (A15), gives the polarization factor. However, the expression (5) or (6) should be used as the polarization factor when the monochromator is set after the specimen crystal.

#### Reference

AZAROFF, L. V. (1955). *Acta Cryst.* **8**, 701–704.

### Notes and News

*Acta Cryst.* (1982). **A38**, 288

#### Seventh European Crystallographic Meeting Book of Abstracts

The Seventh European Crystallographic Meeting will take place in Jerusalem, Israel, from 29 August to 3 September 1982. The Book of Abstracts will be available to non-participants at a price of US\$18.00 including airmail postage. Orders, which must include the words 'Book of

Abstracts', should be sent, no later than 1 July 1982, to ECM-7, PO Box 29313, 61292 Tel Aviv, Israel. Either a cheque payable to ECM-7 should accompany the order or payment should be made by bank transfer to ECM-7, Israel Discount Bank, 4 Rothschild Blvd., 66881 Tel Aviv, Account No. 343900.

For further information on the meeting write to ECM-7, PO Box 29313, Tel Aviv 61292, Israel.

### Book Review

*Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.*

*Acta Cryst.* (1982). **A38**, 288

**История кристаллографии. I: С древнейших времен до начала XIX столетия, II: XIX век.** И. И. ШАФРАНОВСКИЙ. (A history of crystallography.

**I: From earliest times to the beginning of the nineteenth century; II: In the nineteenth century.** By I. I. SHAFRANOVSKII.) Pp. 296 (Vol. I), pp. 324 (Vol II). Leningrad: Nauka, 1978 (Vol. I), 1980 (Vol. II). Price 2r 50k (Vol. I), 2r 40k (Vol. II).

These two volumes (in Russian) contain a comprehensive account of the development of the science of crystals from the earliest times until 1912. They are a pleasure to read – in contrast to the often very difficult writings of the great figures themselves. Professor Shafranovskii is immersed in European culture (he gives his own translations from the *Odyssey*) and he puts life and colour into many prominent people who were otherwise mere names (Capeller, Gadolin, Wollaston, V. Goldschmidt, Steno, Romé de L'Isle, to name only a few). The personalities are treated in their own intellectual and physical surroundings and retrospective nationalism is

absent. The introduction discusses the relationship of crystallography to other sciences and raises contemporary questions about its development in modern times.

Shafranovskii quotes extensively from previous historians of crystallography [Carl Marx, author of *Geschichte der Kristallkunde*, Karlsruhe and Baden (1825), and H. Metzger, *La Genèse de la Science des Cristeaux*, Paris (1918)] stimulating his readers to look back to them. He follows their lead in passing from organising the material first around the gifted individuals and then in later periods around the main topics, such as mathematical crystallography, crystal physics and crystal chemistry, with individuals in a more subordinate role as the subject of crystallography gathered momentum.

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