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Données cristallographiques sur quelques dérivés de la phénothiazine utilisés en pharmacologie. Par PIERRE MARSAU et JACQUES HOUSTY, *Laboratoire de Cristallographie, Faculté des Sciences de Bordeaux-Talence (Gde), France*

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(Diméthylamino-2'-méthyl-2')-éthyl-10-phénothiazine (chlorhydrate)

Ce composé est connu en pharmacie sous le nom de Phénergan.

Les cristaux utilisés sont obtenus à partir d'une solution dans le chlorobenzène; ils sont prismatiques, allongés suivant [010].

$$\begin{aligned} a &= 15,54 \pm 0,05 \text{ \AA} \\ b &= 8,37 \pm 0,03 \\ c &= 15,60 \pm 0,05 \\ \beta &= 122^\circ \end{aligned}$$

Nombre de molécules dans la maille: 4
Densité calculée: 1,24
Groupe spatial: $P2_1/c$

(Diméthylamino-2'-méthyl-2')-éthyl-10-phénothiazine (bromhydrate)

Cristaux obtenus par évaporation d'une solution dans le dichloro-1,2-éthane.

Direction d'allongement [001]. Cristaux prismatiques.

$$a = b = 20,70 \pm 0,05 \text{ \AA} \quad c = 7,98 \pm 0,03 \text{ \AA}$$

Nombre de molécules dans la maille: 8
Densité calculée: 1,42
Groupe spatial: $I\bar{4}$

(Diéthylamino-2'-éthyl-1')-10-phénothiazine (chlorhydrate)

Ce composé est connu en pharmacie sous le nom de Diparcol.

Les cristaux utilisés ont été obtenus à partir d'une solution dans le chloroforme. Direction d'allongement [100]. Cristaux prismatiques.

$$\begin{aligned} a &= 7,37 \pm 0,03 \text{ \AA} \\ b &= 17,33 \pm 0,05 \\ c &= 15,43 \pm 0,05 \\ \beta &= 99^\circ 30' \end{aligned}$$

Nombre de molécules dans la maille: 4
Densité calculée: 1,15
Groupe spatial: $P2_1/c$

(Diéthylamino-2'-méthyl-2')-éthyl-10-phénothiazine (chlorhydrate)

Ce composé est connu en pharmacie sous le nom de Parsidol.

Les cristaux utilisés ont été obtenus à partir d'une solution dans le chloroforme. Direction d'allongement [100]. Forme prismatique.

$$\begin{aligned} a &= 8,82 \pm 0,03 \text{ \AA} \\ b &= 14,43 \pm 0,05 \\ c &= 14,62 \pm 0,05 \\ \beta &= 99^\circ 15' \end{aligned}$$

Nombre de molécules dans la maille: 4
Densité calculée: 1,27
Groupe spatial: $P2_1/c$

Methoxy-3-(diméthylamino-3'-propyl)-10-phénothiazine (maléate acide)

Ce composé est connu en pharmacie sous le nom de Mopazine.

Cristaux en plaquettes, allongés suivant [001], obtenus à partir d'une solution dans le dichloro-1,2-éthane.

$$\begin{aligned} a &= 19,00 \pm 0,05 \text{ \AA} \\ b &= 19,91 \pm 0,05 \\ c &= 11,21 \pm 0,03 \end{aligned}$$

Nombre de molécules dans la maille: 8
Densité calculée: 1,33
Groupe spatial: $Pbca$

Tous ces composés appartiennent à une longue série de produits utilisés en pharmacologie pour leur action sur le système nerveux central (neuroleptiques, antiparkinsoniens) et parfois aussi comme anti-histaminiques.

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A Monte Carlo method for the calculation of the transmission factors of crystals of any shape and absorption power. By A. ALBERTI, *Centro di Calcolo Elettronico dell'Università di Modena, Italy* and G. GOTTARDI, *Istituto di Mineralogia dell'Università di Modena, Italy*

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In the derivation of structure factors from intensities, the major difficulty arises in the calculation of the transmission factor, given by the formula

$$T_{hkl} = \frac{1}{V} \int_V \exp(-\mu l) dV,$$

where V is the volume of the crystal, μ is the linear absorption coefficient (cm^{-1}), l is the length of the X-ray path from the crystal surface to the infinitesimal volume dV (incident beam) plus the distance from the infinitesimal volume dV to the crystal surface (diffracted beam); the integral is extended to the whole volume of the crystal.

It is possible to calculate such an integral by a very simple method, the application of which is limited neither by the shape of the crystal nor by its absorption power. The precision of the result can be fixed at will. The method of calculation is suitable for computer programming.

The principles of this method are as follows:

- (1) Preliminary operations: the equations of the crystal faces, of the incident beam and of the diffracted beam must be given in cartesian coordinates.
- (2) A point is chosen at random inside the volume of the crystal (this is why the method is a Monte Carlo one).
- (3) One calculates the length of the X-ray path from the crystal surface to the point (incident beam) and from the point to the crystal surface (diffracted beam).
- (4) The value of $\exp(-\mu l)$ is calculated and memorized.
- (5) Another point is chosen at random, the corresponding value of $\exp(-\mu l)$ is calculated and memorized, and so on.
- (6) After values of $\exp(-\mu l)$ have been obtained up to a predetermined number (100 in our program), a first average value, A_{100} , is calculated along with the r.m.s. deviation σ . Since the r.m.s. deviation $\sigma(N)$ of the average of N values is

$$\sigma(N) = \sigma/\sqrt{N}$$

one can deduce the number N of $\exp(-\mu l)$ -values which must be calculated to obtain a new average with a predetermined r.m.s. deviation $\sigma(N)$. The calculations of $\exp(-\mu l)$ -values are continued until N such values have been collected, and the final average is the required transmission factor.

The six steps outlined above are sufficiently clear as a general description of the method, but to make its application easier, it is well to explain steps (1), (2), and (3) in greater detail. No further explanation seem to be necessary for steps (4), (5), and (6).

In programming our calculation we use three coordinate systems one after the other: the first, whose axes are xyz , is the direct reference system, which in general is non-orthogonal; the second, whose axes are $x_0y_0z_0$, is orthogonal, where $x_0 = x$, y_0 is the normal to x in the plane xy ; the third, whose axes are $x_a y_a z_a$, is again orthogonal, where x_a is the projection of the incident beam on the reflexion plane, and z_a is the normal to the reflexion plane. Obviously the first two reference systems are valid for any diffraction, whereas the third varies according to the diffraction in question.

At the beginning, the first system (x, y, z) is used to obtain the coordinates of the crystal vertices, the equations of the crystal faces, the equation of the conic surface including all possible incident beams and the equation of the conic surface including all possible diffracted beams of a selected diffraction triplet. After that, all these coordinates and equations are transformed to the second (orthogonal) system $x_0 y_0 z_0$.

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The α_1, α_2 splitting correction for non-integrated Weissenberg X-ray intensity photographs. By E. G. BOONSTRA, National Physical Research Laboratory, Council for Scientific and Industrial Research, P.O. Box 395, Pretoria, South Africa

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The diffraction spots recorded with a non-integrated Weissenberg camera are generally split owing to the α_1, α_2 doublet of the characteristic $K\alpha$ X-ray line. Rae & Barker

The equations of the two straight lines which are the intersections of the incident-beam-cone and the diffracted-beam-cone are then deduced. The resultant coordinates and equations are then further transformed to the system $x_a y_a z_a$. A point O_1 is chosen at random inside the crystal volume. The origin of the system is set at O_1 . Now the incident and the reflected beams are lying in the $x_a z_a$ plane. The coordinates of the points along the incident beam where it meets each of the crystal faces (produced if necessary) are calculated; only the nearest point is relevant; the length of the path of the incident beam is calculated; the same is done for the diffracted beam. The value of $\exp(-\mu l)$ is now readily calculated. The calculation continues as indicated in steps (4), (5), and (6).

On this basis a FORTRAN program has been compiled, which is suitable for crystals of any absorption and form (provided they have no re-entrant angles) and for intensities measured from Weissenberg and Buerger photographs. On an IBM 7094 computer the time needed for assemblage is about two minutes, the time needed to calculate one transmission factor for a crystal of rather simple form (6 faces, maximum length 0.2 mm) with a r.m.s. error of 3% is about 14 seconds. The computing time is proportional to the square of the precision required, to the number of the crystal faces and to μ times the dimensions of the crystal. The program can easily be adapted for use with other experimental data, or with crystals with re-entrant angles, or with curved boundaries.

Our method of calculating transmission factors has some features similar to the method of Busing & Levy (1957). Recently Coppens, Leiserowitz & Rabinovich (1965) and, a few months later, Wuensch & Prewitt (1965) have re-described the Busing & Levy (BL) method, in a way suitable for general application. The BL method differs from ours mainly in that the X-ray path is calculated for a regularly spaced grid of points. The precision obtained is known only at the end of the calculation, and, if greater precision is needed, the calculation must be done again. With our method the precision is predetermined at will.

As far as the difficulty of programming is concerned, our method is very simple. The BL method with its Gaussian quadrature seems to be more complicated from this point of view. The computing time of the BL method could be shorter, but we are unable to predict this with certainty, as until now a general program of the BL method is not available to us. In any case our program is not very time-consuming.

References

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(1961) studied microphotometer traces of such spots and have derived a correction factor $C(\theta)$ which is applied to the measured peak height to yield the integrated intensity