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Determination des mailles et groupes spatiaux de quelques derives anthracèniques.

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Ethyl 9-cyano 10-anthracène $C_{17}H_{13}N$

Le composé se présente sous forme de fines plaquettes jaunes de 0,2 mm. d'épaisseur très propres à l'examen aux rayons X.

Les paramètres de maille déterminés à l'aide de clichés de De Jong et de Bragg sont les suivants:

$$a=16{,}43,\ b=8{,}50,\ c=8{,}70\ \text{Å};\ \beta=91°\ 30'.$$

Ce cristal appartient au système monclinique, la maille contient 4 molécules et la densité calculée est: $d=1{,}26$ g.cm.$^{-3}$. Le groupe spatial est $P2_1/c$.

Cyano 9-dihydro 9-10 anthracène $C_{15}H_{11}N$

Le cyano 9-dihydro 9-10 anthracène qui cristallise sous forme de très belles aiguilles incolores de 0,3 mm. de diamètre a pour paramètres de maille:

$$a=15{,}15,\ b=21{,}90,\ c=6{,}77\ \text{Å}.$$

Ce cristal de symétrie orthorhombique appartient au groupe spatial *Pbca*. Le nombre de molécules par maille est $z=8$ et la densité calculée est: $d=1{,}20$ g.cm.$^{-3}$.

Ethoxy 9-anthracène $C_{16}H_{14}O$

Les cristaux d'ethoxy 9-anthracène d'apparence incolore appartiennent au système orthorhombique. Ils ont pour paramètre de maille a, b, c tels que:

$$a=13{,}69,\ b=9{,}48,\ c=8{,}66\ \text{Å}.$$

Le groupe spatial est *Pbcm*. La maille contient 4 molécules et la densité est calculée égale à $d=1{,}30$ g.cm.$^{-3}$.

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The sensitivity of the correction for extinction in crystals using polarized X-rays and neutrons.

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1. Introduction

Chandrasekhar (1956, 1960) has given a method of correcting X-ray structure factors for extinction in crystals. The method has since been extended (Chandrasekhar & Weiss, 1957) to cover the extinction correction of neutron magnetic structure factors.

For the former case Chandrasekhar (1960) states that the method is 'more powerful the greater the value of θ'. For the latter case no attempt is made to suggest which reflections would be the most sensitive.

In view of the great interest in determining extinction effects, it seems to be worth while to consider the question of sensitivity more carefully.

The notation used here is that used by Chandrasekhar (1960) and Chandrasekhar & Weiss (1957).

2. Calculation of the sensitivity

In the case of X-ray diffraction the amount of extinction can be determined from the measured values of the ratio

$$z=\varrho'_{\varphi}/\varrho'_{\perp}, \tag{1}$$

where $\varrho'_{\perp}$ is the integrated intensity of an X-ray reflection when the incident beam is polarized perpendicular to the plane of incidence, ϱ'_{φ} is the integrated intensity of the same reflection when the incident beam is polarized at an angle φ with respect to the plane of incidence. The natural criterion for the sensitivity of this method is $\partial z/\partial\beta$, i.e. the relative change in z produced by a change in the quantity β, which contains the extinction coefficient. This derivative, which can easily be formed from equation (9) of Chandrasekhar (1960), is

$$\frac{\partial z}{\partial\beta}=\frac{\alpha|F|^2\cos^2\varphi}{(\alpha-|F|^2\beta)^2}\left[\cos^2 2\theta-\cos^4 2\theta\right]. \tag{2a}$$

We have to consider how this derivative depends on θ. This dependence does not lie in the last factor of (2a) alone, since α and β are also functions of θ. α is the same for both primary and secondary extinction:

$$\alpha=\left(\frac{Ne^2}{mc^2}\right)^2\lambda^3\frac{\int\exp\left[-\mu r\right]dV}{\sin 2\theta} \tag{3}$$

β is different for the two kinds of extinction:

$$\beta_{\text{prim.}}=\left(\frac{Ne^2}{mc^2}\right)^4\frac{\lambda^5 t_0^2}{3}\frac{\int\exp\left[-\mu r\right]dV}{\gamma_0^2\sin 2\theta}, \tag{4}$$

$$\beta_{\text{sec.}}=\left(\frac{Ne^2}{mc^2}\right)^4 g\lambda^6\frac{\int r\exp\left[-\mu r\right]dV}{\sin^2 2\theta}. \tag{5}$$

In equations (3), (4) and (5) not only the trigonometric functions but also the integrals and γ_0^2 depend on θ. The exact dependence of the latter two can be given if we know the form and dimensions of the crystal and the value of the absorption coefficient μ.

In the case of neutron diffraction the sensitivity of the method may be given by

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