crystal, we can approximate in formula (29) cos $(2\pi\mathbf{k}\,.\,\mathbf{x})$ by 1 and in this case one obtains

$$I_n(\mathbf{0}) \simeq V f_0^2 \int_{-\infty}^{\infty} V(\mathbf{x}) \exp(\mathbf{0}) \mathrm{d}\mathbf{x} = V^2 f_0^2 \,. \tag{32}$$

The value of the top intensity therefore can vary between $V^2 f_0^2 \exp(-2W)$ and $V^2 f_0^2$ depending upon the crystal size. In the intermediate region between both limits the top intensity will show a more involved temperature dependence than the exponential one.

The temperature factor of the Bragg reflexion intensity also depends on mechanical distortions. This appears from equation (24). At low temperatures $I_n(\mathbf{0})$ will tend to the temperature independent value

$$I_n(\mathbf{0}) = V f_0^2 \int_{-\infty}^{\infty} V(\mathbf{x}) \mathrm{d}\mathbf{x} \int_{-\infty}^{\infty} \Phi_{\mathrm{me}}(\mathbf{x}, \Delta\mathbf{x}) \exp(2\pi i \mathbf{s}_n \,.\, \Delta\mathbf{x}) \mathrm{d}(\Delta\mathbf{x}) \,. \tag{33}$$

If the crystal is sufficiently large and at high temperatures $I_n(\mathbf{0})$ will tend to

$$I_n(\mathbf{0}) = f^2 V^2 \exp(-2W) \,. \tag{34}$$

In the presence of static mechanical distortions the slope of the ln $I_n(\mathbf{0})$ *versus* T curve increases with the temperature. Anharmonicity also causes an increase of that slope. Anharmonicity studies based on this last effect (following the proposal of Maradudin & Flinn, 1963) have to take into account the former effect also.

In the study of the mechanical distortions by harmonic analysis of the Debye–Scherrer line intensity distributions we have to account apparently for the broadening due to the thermal movement. For the separation of the instrumental broadening from the particle size and the distortion broadening effects one generally uses Stokes's (1948) method. Here the experimental intensity distribution is considered as the convolution of $I_n(\mathbf{s}_0)$ given by equation (24) and that of a reference powder: $I_{n,\mathrm{ref}}(\mathbf{s}_0)$.

The thermal broadening effect is separated automatically from the static mechanical distortion broadening effect, if a mechanical undistorted reference powder is used of the same substance as that subjected to the analysis. Indeed, according to equations (24), (25) and (26) we can write

$$I_n(\mathbf{s}_0) = I_{n,\mathrm{th}}(\mathbf{s}_0) * I_{n,\mathrm{me}}(\mathbf{s}_0) \,, \tag{35}$$

with

$$I_{n,\mathrm{th}}(\mathbf{s})_0 = f_0^2 V \int_{-\infty}^{\infty} V(\mathbf{x}) \exp(2\pi i \mathbf{s}_0 \,.\, \mathbf{x}) \mathrm{d}\mathbf{x} \int_{-\infty}^{\infty} \Phi_{\mathrm{th}}(\mathbf{x}, \Delta\mathbf{x}) \times \exp(2\pi i \mathbf{s}_n \,.\, \Delta\mathbf{x}) \mathrm{d}(\Delta\mathbf{x}) \tag{36}$$

and

$$I_{n,\mathrm{me}}(\mathbf{s}_0) = \int_{-\infty}^{\infty} \exp(2\pi i \mathbf{s}_0 \,.\, \mathbf{x}) \mathrm{d}\mathbf{x} \int_{-\infty}^{\infty} \Phi_{\mathrm{th}}(\mathbf{x}, \Delta\mathbf{x}) \times \exp(2\pi i \mathbf{s}_n \,.\, \Delta\mathbf{x}) \mathrm{d}(\Delta\mathbf{x}) \,. \tag{37}$$

We thank Professor A. G. M. Janner for his critical remarks and advice.

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Interpretation of Anomalous Streaks in Crystals of Anthrone

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Streaks on $\{hll\}$ Weissenberg photographs of some anthrone crystals have been explained as being due to disorder in the stacking sequence of a layer structure or to multiple twinning on $(20\bar{1})$. The two views are geometrically identical. With such a model no streaks are either expected or observed on $\{h0l\}$ Weissenberg photographs.

Introduction

Flack (1968, 1970) and Glazer (1968, 1970) have recently made an extensive study of short-range order, thermal vibration and expansion of pseudosymmetric and mixed crystals of some small organic molecules. For example, stationary-crystal photographs of anthrone (I) taken with white plus characteristic X-radiation show layers of diffuse scattering corresponding to $k=\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$. This diffuse scattering has been interpreted in terms of domains of short-range order ori-

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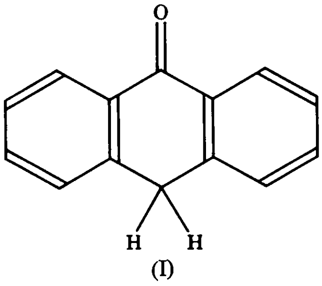
ginating in non-centrosymmetric molecules being located at statistical centres of symmetry of the lattice. (Anthrone $P2_1/a$, $Z=2$). These diffuse layers have been observed from all solution-grown crystals of anthrone so far examined and from some mixed crystals of anthrone and (isostructural) anthraquinone. Glazer (1968, 1970) finds similar effects with phenazine and *N*-oxyphenazine.



(I)

In addition to the diffuse layers, Lonsdale, Nave & Stephens (1966) observed streaks lying perpendicular to $(20\bar{1})$ on $\{h1l\}$ Weissenberg photographs of some crystals of anthrone (see Fig. 19(*b*) of Lonsdale, Nave & Stephens, 1966). Lonsdale *et al.* (1966) interpreted the streaking as 'some special form of limited disorder, involving short-range order such as platelets parallel to $(20\bar{1})$ which have internal order, but with disorder of successive platelets'. In the present communication this interpretation is amplified by taking account of the specific geometric structure of crystalline anthrone.

Experimental

Crystals of anthrone were grown from solutions of ethanol or glacial acetic acid by slow cooling, from solutions of diethyl ether by slow evaporation or from the molten state. These crystals, which were needles or laths elongated along [010], were examined by taking $\{h0l\}$ and $\{h1l\}$ Weissenberg photographs with Cu $K\alpha$ radiation. Approximately 35 crystals were investigated. It was found that streaking normal to $(20\bar{1})$ frequently occurred on $\{h1l\}$ but never on $\{h0l\}$ Weissenberg photographs. The relative intensity and extent of the streaks varied from crystal to crystal but they always occupied the same positions in reciprocal space. All crystals producing streaks were twinned with $(20\bar{1})$ as twin plane but in some twinned crystals streaking was not observed. Crystals grown from diethyl ether solution never showed streaking.

Fig. 1(*d*) shows the reciprocal net derived from the $\{h1l\}$ Weissenberg photographs. It is not immediately clear whether the streaks are planes of limited extent or lines in reciprocal space. They are in fact lines. This has been verified with stationary-crystal photographs using white plus characteristic X-radiation. Full details are given by Flack (1968).

A model for disordered anthrone

Fig. 1(*a*) shows a projection on (010) of the crystal structure of anthrone. (The hydrogen atoms have been omitted.) The structure may be considered as being built up of identical layers of molecules stacked parallel to $(20\bar{1})$. Now suppose that in building up the structure, 'mistakes' occur in the position of one layer relative to the next. In Fig. 1(*a'*) we show an alternative stacking sequence which constitutes a 'mistake'. It is obvious that the structures [Fig. 1(*a*) and (*a'*)] are mirror images of each other in $(20\bar{1})$, the twin plane.

A disordered crystal will be produced if the stacking of the layers takes place with an irregular mixture of the two stacking sequences. Such a crystal may also be considered as being formed by multiple twinning on $(20\bar{1})$.

Scattering from the disordered crystal

Wilson (1962) has given a mathematical treatment of the X-ray scattering to be expected from a layer-structure with irregular variations in the stacking sequence. His model is essentially the same as that postulated here for a disordered crystal of anthrone. Wilson has shown that those reflexions whose structure factors are affected by the mistake in question, will be drawn out in reciprocal space in a direction perpendicular to the layers. Other reflexions will be unaffected. In order to apply these results to the disordered model of anthrone, the assumption is made that $(20\bar{1})$ is a mirror plane in the (010) projection. This implies that $a=2c$ and that the values of the structure factors for the reflections $2h,k,l$ and $2l,k,h$ are identical. The data given by Flack (1968, 1970) indicate approximate mirror symmetry across $(20\bar{1})$ in the (010) projection.

As the structures in Fig. 1(*a*) and (*a'*) represent stacking sequences with 'no mistakes' and 'all mistakes' respectively, a comparison of their reflexions in reciprocal space will show how the values of the structure factors are affected by the introduction of mistakes. In Fig. 1(*b*), (*b'*), (*c*) and (*c'*) are shown the $\{h0l\}$ and $\{h1l\}$ sections of reciprocal space.

Consider firstly the $\{h0l\}$ sections. Owing to the $(20\bar{1})$ mirror symmetry, these are identical. Thus there should be no elongation of the $h0l$ reflexions, in agreement with the experimental observations. The structure factors in the $\{h1l\}$ sections show differences. These will result in elongation of some $h1l$ reflexions, possibly into streaks as shown in Fig. 1(*d'*). A comparison of Fig. 1(*d*) and (*d'*) shows that the diffraction effects of the postulated model agree with the experimental observations.

Streaking on $\{h2l\}$, $\{h3l\}$,... should be similar to that in $\{h1l\}$. The presence of lines in $\{h2l\}$ perpendicular to $(20\bar{1})$ was evident on the stationary-crystal photographs using white plus characteristic radiation. The elongation of reflexions was also faintly visible on $\{h2l\}$ Weissenberg photographs. Streaking has never been observed on higher layers. This is most likely due

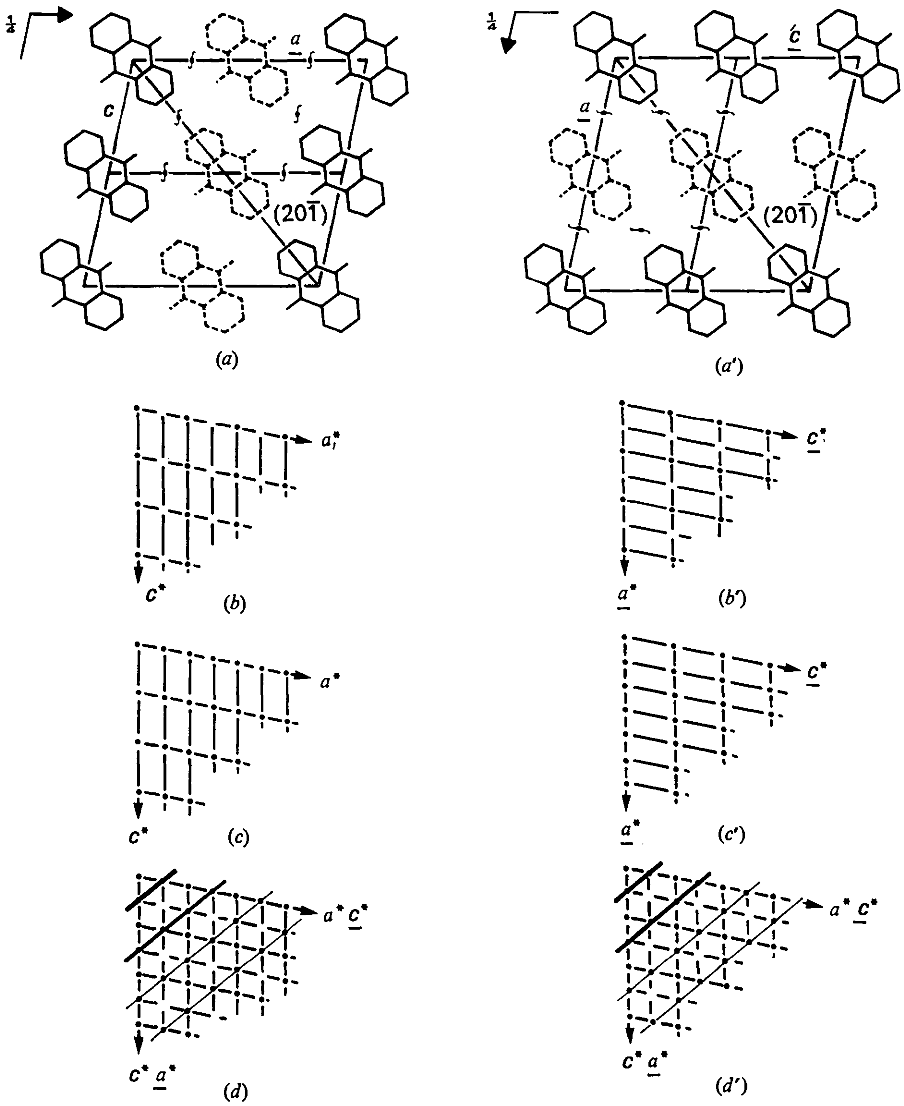


Fig. 1. (*a*) Projection of crystal structure of anthrone on (010). (*a*′) Mirror image of 1(*a*) in the twin plane (20$\bar{1}$). (*b*) and (*b*′) $\{h0l\}$ reciprocal-lattice sections of structures 1(*a*) and 1(*a*′) respectively. (*c*) and (*c*′) $\{h1l\}$ reciprocal-lattice sections of structures 1(*a*) and 1(*a*′) respectively. (*d*) $\{h1l\}$ section observed from a crystal of anthrone. (*d*′) $\{h1l\}$ section deduced for a disordered crystal. (Underlining of axes indicates twin orientation.)

to the general weakening of intensity of reflexions at high θ angles.

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