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Diffuse layers in anthrone photographs. By SURENDRA NATH SRIVASTAVA, *Department of Physics, Allahabad University, Allahabad, India*

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The X-ray rotation photographs about the b axis of anthrone present a peculiar appearance of alternate diffuse and sharp layer lines. Anthrone belongs to the space group C_{2h}^5–$P2_1/a$, with cell constants (Srivastava, 1959)

$$a = 15{\cdot}80,\ b = 3{\cdot}998,\ c = 7{\cdot}86\ \text{Å};\ \beta = 101°\ 40'.$$

Density as determined by flotation is $1{\cdot}33_2$ g.cm.$^{-3}$, and the calculated value on the basis of two molecules per unit cell is $1{\cdot}33_5$ g.cm.$^{-3}$. The structural formula is shown in Fig. 1, and shows that the molecule of anthrone does

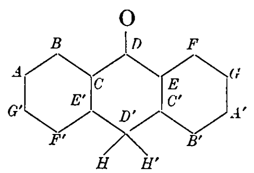

Fig. 1. *Molecule of anthrone*

not possess the centre of symmetry. There thus cannot be only two asymmetric molecules per unit cell. However this point can be explained. First let us consider the diffuse layer lines, which occupy a position that would be occupied if the b axis were doubled ($= 7{\cdot}996$ Å), and therefore indicate some disorder perpendicular to the b axis. Suppose the molecule to consist of two parts, one part being the oxygen and two hydrogen atoms, and the second part being the anthrone molecule without these atoms. The second portion has a centre of symmetry and can therefore belong to the above space group with only two molecules per unit cell. There can be two ways in which the first part can be attached to the second, i.e. either the oxygen atom is attached to D and the hydrogen atoms to D' or vice versa. Let us designate the first type of molecule as A and the second as B. The following possible types of arrangements in an anthrone crystal are considered.

(1) All the molecules in the crystal are of type A.

(2) In the row of molecules parallel to [010] direction, molecules alternate regularly as $ABABABABABAB\ldots$.

(3) The arrangement of the molecule along a row parallel to [010] is same as in the arrangement (2), but in any layer parallel to the (010) plane both types of molecules occur with equal probability.

The first type of the arrangement is untenable, since that would give only regular layer lines corresponding to the $b = 3{\cdot}998$ Å and would give no diffuse layers and the space group will be Pa.

The second type of the arrangement would correspond to a b axis of twice its present value. The scattering of X-rays along the directions of the odd layers would be only due to the contributions from oxygens and hydrogens attached to the central ring; the second portion of the molecule, being centrosymmetric, would not contribute at those places. Thus the intensities of the odd layers would be much smaller than the even layers, and the odd layers would not be diffuse.

In the arrangement (3) let us assume that the molecule at the origin is of type A. In the arrangement of either (1) or (2) all the molecules which lie in the layer parallel to the (010) plane will be of type A. but if some disorder occurs then there would be some type B molecules, and by another mistake the molecules would revert to type A. In this way there would be random distribution of the A and B type of molecules in the plane parallel to (010). The integral breadth would be $\alpha/(1-\alpha)$, where α is the probability of the mistake occurring in one direction (Wilson, 1949). Therefore if α exceeds $\frac{1}{3}$, the integral breadth would be greater than $\frac{1}{2}$, and thus the reciprocal-lattice points would diffuse to such an extent that they would overlap. If therefore the disorder occurs parallel to (010) then the reciprocal-lattice points would smear to form continuous diffuse regions. At the places where strong spectra are expected, we would expect diffuse patches of sufficient intensity. These have been observed, and hence the arrangement (3) is the only one which explains the X-ray scattering satisfactorily. Since there is equal probability of the occurrence of A and B type of molecules along a plane parallel to (010), it would mean statistically that half of an oxygen and half of two hydrogen atoms are attached to the two carbon atoms D and D' of the central ring of the anthrone molecule. In this manner the unsymmetrical molecules have achieved the statistical symmetry in the crystal of anthrone, and hence the absent spectra can be successfully accounted for.

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References

SRIVASTAVA, S. N. (1959). *Indian J. Phys.* **33**, 456.
WILSON, A. J. C. (1949). *X-ray Optics*. London: Methuen.