

of varying  $n$ , and that the method has not the sensitivity claimed for it. The sensitivity would be still further reduced if, as often happens, a face is growing at less than the maximum rate permitted by diffusion, and the contours are less crowded.

It is suggested that, in view of these comments, an explanation has been found for Goldsztaub & Kern's negative result.

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## The Space Group of Anthraquinone

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The weak forbidden reflexions which were observed by Sen in the zero-layer [010] Weissenberg photograph of anthraquinone and which prevented him deciding on the space group are shown to be due to Renninger reflexions. By applying the statistical tests of Wilson and Howells *et al.* to the ( $hk0$ ) and ( $0kl$ ) projections, the presence of a centre of symmetry is also proved. The space group of anthraquinone is therefore unequivocally established as  $P2_1/a$ .

### Introduction

The crystal structure of anthraquinone,  $C_{14}H_8O_2$ , was determined by Sen (1945) by two-dimensional Fourier synthesis. The pseudo-orthorhombic ( $hk0$ ) (monoclinic ( $h0l$ )) projection was well resolved. On applying Booth's (1945) accuracy test, the value for  $R_1$  for the projection is 0.21, which is a comparatively large figure. Moreover, all the possible reflexions in that projection with  $Cu K\alpha$  were not recorded. It was, therefore, thought worth while to undertake a refinement of the structure by a three-dimensional Fourier synthesis. Sen (1940) assigned to the crystal the space group  $P2_1/a$ , but in his later work (Sen, 1948) mentioned the observation of a few weak forbidden reflexions ( $h0l$  with  $h$  odd) on a strong Weissenberg photograph, and this led him to ascribe  $P2_1$  as the correct space group. In the present investigation a critical re-examination of the space group was therefore undertaken.

### Forbidden reflexions

An over-exposed normal-beam zero-layer-line Weissenberg photograph about [010] was taken, using unfiltered  $Cu$  radiation, in order to record the forbidden reflexions observed by Sen. In this photograph a few more reflexions of the same type appeared. All these spots were sharper than the normal reflexions, and, moreover, even the strongest of them was not associated with the usual reflexion due to  $Cu K\beta$  whereas every equally intense normal  $K\alpha$  reflexion had its  $K\beta$  reflexion. These reflexions were, therefore,

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suspected of being due to double reflexions from two strong reflecting planes, as suggested by Renninger (1937). By construction in the reciprocal lattice these reflexions were found to be due to double reflexions, as shown in Table 1. In all cases but the last one the

Table 1

Observed forbidden reflexion	Pairs of planes giving rise to the corresponding forbidden reflexion
(101)	( $11\bar{3}$ , $0\bar{1}4$ ), ( $211$ , $\bar{1}10$ ), ( $524$ , $\bar{4}25$ )
(102)	( $212$ , $\bar{1}10$ ), ( $11\bar{1}$ , $0\bar{1}3$ ), ( $413$ , $\bar{3}11$ )
( $\bar{1}02$ )	( $321$ , $\bar{4}21$ ), ( $013$ , $\bar{1}11$ )
(302)	( $512$ , $\bar{2}10$ ), ( $211$ , $\bar{1}11$ )
(502)	( $211$ , $\bar{3}11$ ), ( $210$ , $\bar{7}12$ )
(103)	( $112$ , $0\bar{1}1$ ), ( $614$ , $\bar{5}17$ )
( $\bar{3}03$ )	( $110$ , $\bar{4}13$ )

contribution is observed to be from more than one pair, and estimates of intensity agree with the sum of the intensities expected from the various pairs that produce any particular reflexion.

### Statistical tests for centrosymmetry

The presence of the centre of symmetry required by this space group was confirmed by the statistical methods of Wilson (1949) and Howells, Phillips & Rogers (1950). Normal-beam Weissenberg photographs about the monoclinic [100] and [001] axes were taken with unfiltered  $Cu$  radiation. Integrated intensities of the spots were measured with a Moll recording microphotometer and were corrected for the angle factor only. Relative values of the structure factors were

calculated and were put on an absolute scale by comparing with some of the  $(h0l)$  planes whose structure factors were given by Sen (1948).

The intensities with the corresponding structure factors were divided into groups of different  $\sin \theta$  range and Wilson's ratios ( $\rho = \langle |F|^2 \rangle / \langle I \rangle$ ) for the respective groups, and Rogers'  $N(z)$  values for different values of  $Z$  were obtained. A weighted average of all these  $\sin \theta$  groups was taken in the usual manner.

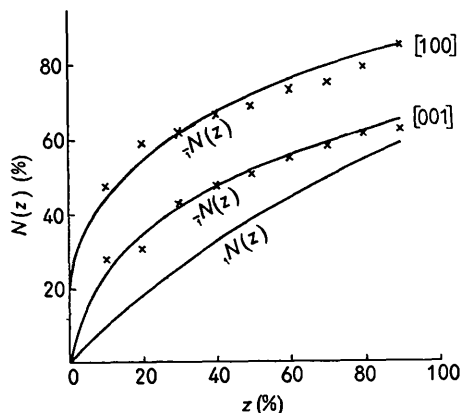


Fig. 1.  $N(z)$  values for the [100] and [001] projections of anthraquinone. Successive  $\bar{N}(z)$  curves are displaced 20% vertically.

The weighted  $N(z)$  averages are plotted in Fig. 1. The continuous curves are the theoretical ones.

### Results

From the above, Wilson's ratio for the  $(hk0)$  projection was found to be 0.610 and for the  $(0kl)$  projection it was 0.587. These values agree reasonably well with the theoretical value of  $2/\pi = 0.636$  for the centrosymmetric case. From the figure it is clearly observed that the experimental values of  $N(z)$  agree very well with the theoretical curve for the centrosymmetric case. Thus the existence of the centre of symmetry necessary for the space group  $P2_1/a$  is definitely established.

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## Short Communications

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

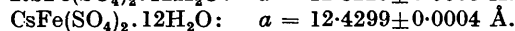
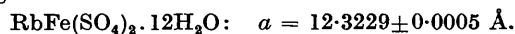
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**Lattice constants of rubidium and cesium iron alums.** By HAROLD P. KLUG, *Mellon Institute, Pittsburgh 13, Pa., U.S.A.*

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Several years ago, during a study of iron alums, precision lattice-constant determinations were made on rubidium and cesium iron alums at  $25 \pm 0.1^\circ$  C. Since these data may be of interest to some investigators they are being briefly reported at this time. Details of the X-ray techniques used in these determinations have been described earlier (Klug & Alexander, 1940). The lattice constants reported below are the mean of six and four values

respectively, together with the average deviation of a single result from the mean.



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