LETTERS TO THE EDITORS

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Crystal Structure of Rhombohedral Sulphur

THE allotropic form of sulphur first discovered by Engel¹ has been variously termed Engel's sulphur, S_8 , S_p , trigonal sulphur, and rhombohedral sulphur. The molecule was shown to be hexameric by Aten². Friedel³ found the crystals were hexagonal prisms terminated by a flat rhombohedron. Although these crystals are largely converted to a mixture of plastic and orthorhombic sulphur an hour or so after they have been exposed to air or X-rays, Frondel and Whitfield⁴ were able to determine the hexagonal lattice constants, show that the symmetry axis was three-fold, and demonstrate the absence of vertical planes of symmetry; the lattice constants, combined with the observed density¹, give 18 sulphur atoms per unit cell. The quality of their photographs was such that they were unable to determine whether the lattice mode was hexagonal or rhombohedral. Their X-ray study, however, combined with the morphological observations, established the point group as $C_{3i}-\bar{3}$, and Donnay⁵ later pointed out that on purely morphological grounds the lattice is rhombohedral and that the space group is thus probably $C'_{3i}-R\bar{3}$ (No. 148).

By taking rotation and small oscillation-range Weissenberg photographs around a and c , each with a different crystal, we have verified directly that the lattice is indeed rhombohedral. For the triply primitive hexagonal cell, we find the provisional values $a = 10.83$ Å. and $c = 4.26$ Å., in satisfactory agreement with Frondel and Whitfield's values of 10.9 kX. and 4.26 kX. The general position of $C'_{3i}-R\bar{3}$ is six-fold; the primitive rhombohedral cell accordingly contains one molecule of S_8 .

There are 31 unique $(hk.l)$ reflexions accessible to $K\alpha$ copper radiation, and 25 of these have been

observed. By the use of intensities estimated with the multiple film technique together with signs for the structure amplitudes obtained with the aid of a map of the molecular structure factor, we have prepared the projection of electron-density on (00.1), Fig. 1. The x and y parameters measured from this projection must be regarded as preliminary because neither series-termination effects nor errors due to absorption have been taken into account.

Our $(0kl)$ photographs are somewhat poorer in quality than our (hkl) photographs. Qualitative intensity considerations suggest a value of the z parameter of about 1/10. The fact that z is not zero means that S_8 molecules are staggered rings with symmetry $D_{3d}-3m$. The approximate bond-length¹ is 2.0 Å., the bond-angle about 100°. We expect to obtain more precise values for these and other angles and distances of interest when the structure has been more completely refined.

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The Four Elastic Constants of Diamond

THE thermal scattering of light in diamond has been studied in great detail by R. S. Krishnan¹ and by V. Chandrasekharan². These authors pointed out that the frequency shifts observed for the Brillouin components are not in good agreement with the values calculated using the elastic constants data of Bhagavantam and Bhimasenachar³. The values of the elastic constants have since been determined by Prince and Wooster⁴ and recently much more accurately by McSkimin and Bond⁵. McSkimin and Bond's values do not agree with those of Bhagavantam and Bhimasenachar and of Prince and Wooster, especially as regards C_{12} and C_{44} . Using the values of McSkimin and Bond, the frequency shifts of the Brillouin components for the various orientations studied by Chandrasekharan with the bigger spectrograph were calculated, but the agreement with the experimental values was still unsatisfactory. We have therefore evaluated the elastic constants of diamond directly from the observed frequency shifts⁶.

To achieve this, three values of the frequency shifts must be assumed. For convenience, the shifts of the longitudinal component arising from the elastic waves moving approximately along the direction $[144]$, which is inclined at about 10° to $[011]$, and the longitudinal and transverse components of the elastic waves approximately along the direction $[811]$, which is inclined at about 10° to $[100]$, have been taken and, by a perturbation procedure⁷, the elastic constants have been calculated. The values are $C'_{11} = 94.9$, $C'_{12} = 15.1$ and $C'_{44} = 52.1 \times 10^{11}$. The accuracy is estimated to be 3-5 per cent, chiefly due to the errors possible in the angle of scattering. Using these elastic constants the effective elastic constants and the Brillouin shifts have been calculated for all the orientations and the results are given in Table 1.

Fig. 1. Electron-density projected down the c -axis. Contours drawn at intervals of five electrons per Å.² (zero contour dotted)