SHORT COMMUNICATIONS

The Crystal Structure of Meso-pentane-2, 4-diol Borate

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In the course of a structural investigation of the model substances of polyvinyl alcohol, we have analyzed the crystal structure of meso-pentane-2, 4-diol borate.[1] This compound crystallizes in a monoclinic form, with unit cell dimensions of $a=15.36$ Å, $b=13.39$ Å, $c=7.60$ Å, and $\beta=113.0°$ The systematic absences of the reflections show that the space group is $C\,2/c$ or Cc. As the statistical test of the intensity distributions suggests that there exists a center of symmetry in the crystal, it was decided that the space group was $C\,2/c$. As this compound is very hygroscopic and is easily dissolved in nearly all kinds of solvents, it was very difficult to determine the density of the crystal. However, from the fact that the crystal is a little heavier than water, it is reasonable to consider that there are 8 molecule in the unit cell.

Multiple film equi-inclination Weissenberg photographs about the c axis were taken with CuK_α radiation for layers from 0 up to 6, while the intensities were estimated visually against a standard scale.

The structure was analyzed mainly by the Patterson projection along the c axis. The positional and thermal parameters of each atom so obtained were then refined by the least-square method. The reliability index, R, for (hkl) reflections at this stage of analysis is 18%, omitting the unobserved reflections. The final electron density projection along the c axis is shown in Fig. 1.

Surrounding the center of symmetry, two molecules are hydrogen-bonded, as is shown in Fig. 2, the distance of the hydrogen bond being about 2.8 Å. The boron atom is surrounded by three oxygen atoms, which form an almost equilateral triangle about the boron; these four atoms are nearly coplanar. The two CH groups and the two oxygen atoms are almost on one plane; all the carbon atoms also form a plane. These three planes, namely, the plane containing all the carbon atoms, that containing two CH groups and two oxygen atoms, and that containing the BO_3 group, intersect to form a chair-like structure. The details of the structure analysis will be reported in the near future.

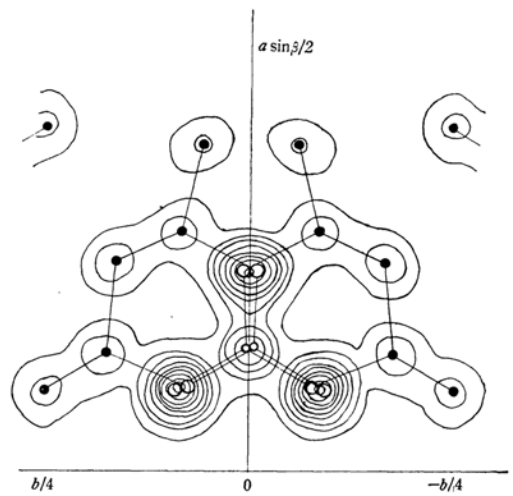

Fig. 1. The final electron density projection on the (001). Contours are in arbitrary unit. Black circles indicate carbon atoms, small open circles indicate boron atoms, and large open circles indicate oxygen atoms.

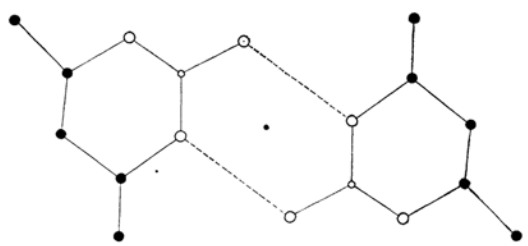

Fig. 2. Two hydrogen bonded molecules. The broken lines indicate the hydrogen bonds, small black circle indicates the center of symmetry. Other circles are as in Fig. 1.

1) E. Nagai, S. Kuribayashi, M. Shiraki and M. Ukita, *J. Polymer Sci.*, **35**, 295 (1959).