The Crystal and Molecular Structure of Disodium β-Glycerolphosphate Pentahydrate [$Na_2PO_4C_3H_5(OH)_2$, $5H_2O$]

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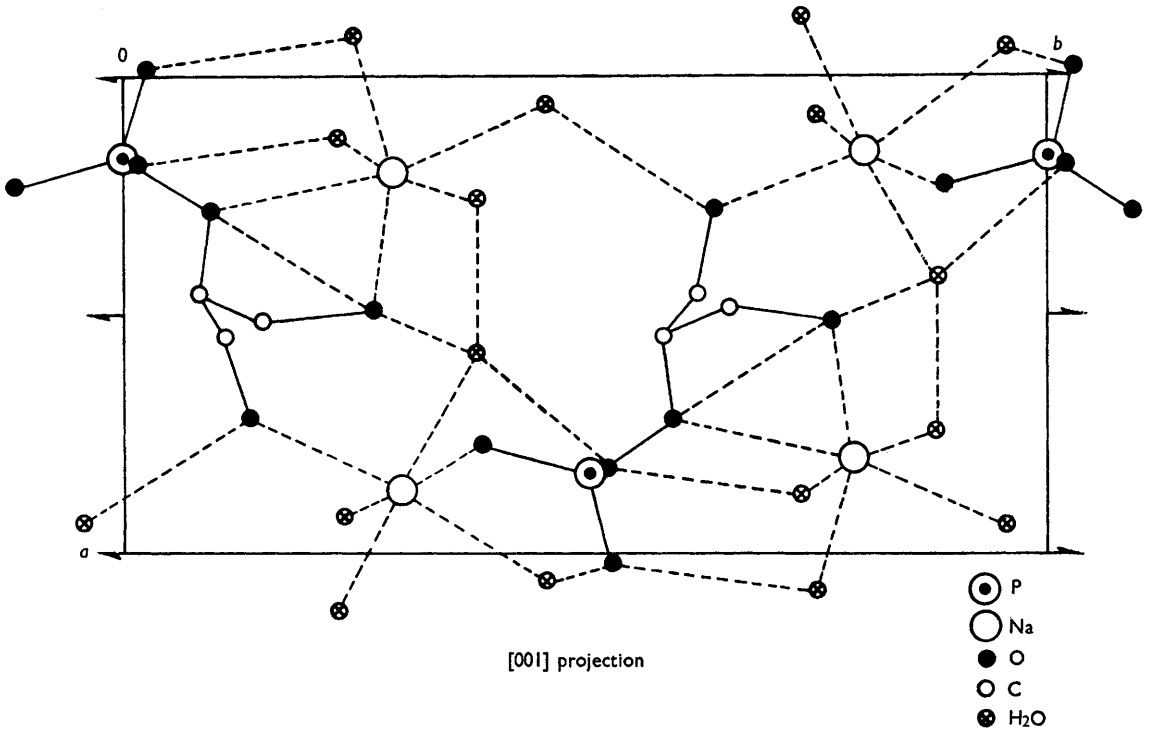
GLYCEROLPHOSPHATES are involved in the biosynthesis and degradation of phospholipids, the synthesis of fats from fatty acids, in the exchange of hydrogen in biological systems, as well as in a variety of other biologically important processes. Since most of these functions involve hydrolysis

of the P–O–C bond at one step or another, precise structural information is significant in understanding the process. The structure of L-α-glycerolphosphorylcholinecadmium chloride trihydrate has been reported by Sundaralingam and Jensen.[1] We give here a preliminary report on the structure of disodium β-glycerolphosphate pentahydrate.

Good crystals of disodium β-glycerolphosphate were obtained by slow recrystallization from water. Preliminary investigation indicated that these were the pentahydrate, and thus in order to prevent possible loss of water during the collection of *X*-ray data, a small crystal was selected and sealed in a glass capillary. The crystal was of approximate uniform cross-section about 0·2 mm. on a side and about 1 mm. long. The crystals are monoclinic, belonging to space group $P2_1$ and have two molecules per unit cell. Unit cell parameters are $a = 7{\cdot}94$, $b = 12{\cdot}10$, $c = 6{\cdot}18$ Å, $\beta = 107°$. Multiple film Weissenberg photographs were taken for intensity measurements. Intensities were measured by scanning with a densitometer reflections that had been integrated in a direction perpendicular to the direction of scanning. Areas under the densitometer tracings were measured with a planimeter. Intensities for 884 independent reflections were measured and used for the structure determination.

Solution of the structure was possible from the Patterson map and successive Fouriers along with the use of a minimum function. It was possible to locate the position of the phosphorus atom first, then several oxygens, the glycerol group, and finally the water oxygens and the sodiums. At this point all except phosphorus and carbons were assumed to be oxygens. Later Fouriers showed sodium atoms as distinguished from oxygens. The present *R*-factor is 13% and refinement is continuing with Busing, Martin, and Levy Least-Squares refinement programme (ORNL–TM–305). The figure shows the [001] projection of the structure. Sodium co-ordination and hydrogen bonding are represented by broken lines. Points of particular interest are the following: each of the phosphate oxygens is involved in hydrogen bonding or co-ordinated to sodium. The bond distances and angles are normal for this stage of refinement when compared with other organic phosphates.[1-3] Both sodium atoms are six-co-ordinated with the Na–O distances from 2·27 to 2·59 Å. A strong network of hydrogen bonding and sodium co-ordination holds the crystal together.



[001] projection

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[1] M. Sundaralingam and L. H. Jensen, *Science*, 1965, **150**, 1035.
[2] M. Sundaralingam and L. H. Jensen, *J. Mol. Biol.*, 1965, **13**, 914, 930.
[3] Chi-Tang Li and C. N. Caughlan, *Acta Cryst.*, 1965, **19**, 637.