

The Crystal Structure of Phosphoric Acid

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The crystal structure of phosphoric acid, H_3PO_4 , has been determined, using X-ray diffraction methods. The unit cell is monoclinic with $a = 5.78 \text{ \AA}$, $b = 4.84 \text{ \AA}$, $c = 11.65 \text{ \AA}$, and $\beta = 95.5^\circ$. The space group is $P2_1/c$ and there are four molecules per unit cell, corresponding to a density of 2.01 g.cm^{-3} .

The positions of the phosphorus and oxygen atoms were derived from Patterson- and Fourier-projections along the a and b axes. The reliability factor R is at this stage about 0.23 for both projections and the structure is being further refined. In Fig. 1 the Fourier projection in direction of the b axis is shown.

Although the structure cannot be discussed in detail at this stage, it appears that the four P—O bonds are all of approximately the same length, not far from the value of 1.56 \AA found by West¹ in the crystal structure of KH_2PO_4 . The PO_4 tetrahedron is fairly regular. Hydrogen bonds hold the molecules together. Two of the oxygen atoms probably take part in two such bonds, whereas the other two seem to participate in only one hydrogen

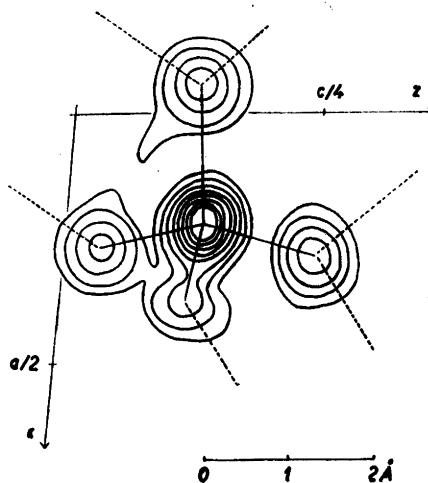


Fig. 1. Electron-density projection along the b axis.

bond. This is indicated by dotted lines in the figure.

A detailed description of the structure will be published at a later date.

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1. West, *J. Z. Krist.* **74** (1930) 306.

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