An X-ray Diffraction Study of the Structure of Vitreous P_2O_5

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Z. Naturforsch. **53a,** 93–104 (1998); received December 22, 1997

Recently, the lengths of the two P-O bonds in the PO_4 tetrahedron were obtained by neutron diffraction of high real-space resolution. By use of the present X-ray diffraction experiments, the P-P distance belonging to pairs of corner-linked PO_4 units is determined. Using this length of (294 ± 2) pm and taking into account the P-O bond distance to the bridging oxygen atom of 158 pm, a mean P-O-P angle of 137° ± 3° is calculated. The reverse Monte Carlo simulations fit the neutron and X-ray structure factors. The P-O-P angle distribution obtained this way possesses a mean angle of 141°. An interpretation of the first scattering peaks is presented by analysing the occupancy and the distances of various coordination shells by use of model configurations. The low occupancy of the first shells allows the application of the schematic hole model of Dixmier. The first X-ray diffraction peak at 13 nm^{-1} is related to the $P\text{-}P_{2nd}$ shell, the shoulder at 20 nm^{-1} arises from the $P\text{-}O_{2nd}$ shell. The most similar crystalline structure with vitreous P_2O_5 is the orthorhombic P_2O_5, form II. But it has more effectively orientated terminal oxygen atoms and, thus, a higher packing than the glass.

Key words: Vitreous P_2O_5; X-ray Diffraction; Short-range Order; Reverse Monte Carlo.

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