Variation in P-O Bonding in Phosphate Glasses

A Neutron Diffraction Study

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Two different lengths of P-O bonds in the PO_4 units of phosphate glasses are found by neutron diffraction experiments of high resolution in real space. The two lengths are related to bonds of the phosphorus atom with the terminal and the bridging oxygen atoms. The mean lengths and widths of both P-O distance peaks change as a function of the glass composition. In a large range, starting from vitreous P_2O_5 up to the pyrophosphate composition, the behavior of the bond lengths is compared with that in the related crystals and with that resulting from ab initio calculations. The bond lengths depend not only on the species of the participating oxygen atoms and on the number of links of the concerning PO_4 unit but also on the number of links of the neighboring PO_4 unit and on the species of the modifier cation.

Key words: Neutron Diffraction; Short-range Order; Phosphate Glasses.