Structural Role of Water in a Sodium Phosphate Glass by Neutron Diffraction

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Neutron diffraction with isotopic H/D-substitution was used to study the network-modifying effect of water in a H_2O-Na_2O-$2P_2O_5$ glass. The resolved fractions of P−O_T and P−O_B bonds and the O−O coordination number indicate similarity to the specifics of a metaphosphate structure. Thus, oxygen of H_2O added ruptures a P−O−P bridge, increasing the number of terminal oxygens. The combined analysis of the first-neighbour peaks in the correlation functions of the hydrogenated and deuterated samples yields H−O distances of 0.101 and 0.157 nm and H−P distances of 0.223 and 0.250 nm. Such distances are well explained with the formation of O−H···O hydrogen bridges. The corresponding O−O distances superpose with the edge lengths of the PO_4 tetrahedra. Significant fractions of short H−H distances typical of water molecules (0.155 nm) or clustering of hydrogen bridges are not detected. The Na−O coordination number of five is similar to that found for the $NaPO_3$ glass.

Key words: Isotopic Substitution; Neutron Scattering; Hydrogen Bridges; Phosphate Glasses.