

The determination of hydrogen positions in superhydrous phase B

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ABSTRACT

Nominally hydrous high-pressure silicate phases such as the superhydrous phase B are of considerable importance for the understanding of the water-cycle between the surface and the interior of the Earth. This study tackles the controversial issue of hydrogen positions in superhydrous phase B, a phase believed to be potentially stable in cold subducting ultramafic slabs. To investigate the nature of hydrogen incorporation into the structure of superhydrous phase B, neutron powder diffraction experiments have been performed. A structural model based on *Pnn2* symmetry has been used for the analysis of the data, which is consistent with earlier spectroscopic studies. Application of Fourier synthesis with subsequent analyses of difference nuclear density maps and Rietveld fits reveal two distinct positions for deuterium, at $4c$ (0.194, 0.052, 0.596) and at $4c$ (0.186, 0.119, 0.388). This unambiguously shows that deuterium lies within large channels, which are formed between the edge-shared octahedra and vertex-linked tetrahedra along the **b**-axis of the structure. These results contrast with recent polarized single-crystal infrared spectroscopy studies where the position of one of two H atoms was estimated to lie close to the octahedral edge of an MgO₆ octahedron, thereby leaving the large structural channel empty.

Keywords: Hydrous magnesium silicates, neutron diffraction, superhydrous phase B, crystal structure, hydrous minerals, determination of hydrogen positions