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LETTER

Crystal chemistry of dense hydrous magnesium silicates: The structure of phase H, $MgSiH_2O_4$, synthesized at 45 GPa and 1000 °C

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ABSTRACT

The crystal structure of the dense hydrous magnesium silicate phase H, $MgSiH_2O_4$, synthesized at 45 GPa and 1000 °C, was investigated by single-crystal X-ray diffraction. Although showing a deterioration process under the X-ray beam, the compound was found to be orthorhombic, space group *Pnnm* ($CaCl_2$-type structure), with lattice parameters $a = 4.733(2)$, $b = 4.3250(10)$, $c = 2.8420(10)$ Å, $V = 58.18(3)$ Å^3, and $Z = 1$. The structure was refined to $R_1 = 0.0387$ using 53 observed reflections [$2\sigma(I)$ level]. Magnesium and silicon were found to be disordered at the same octahedral site (with a mean bond distance of 1.957 Å). Hydrogen was not located in the difference Fourier maps, but it is very likely disordered at a half-occupied 4*g* position. The centrosymmetric nature of the structure of phase H is examined in relation to that reported for pure δ-AlOOH at ambient conditions (non-centrosymmetric, $P2_1nm$), and the possibility that these two compounds can form a solid solution at least at high pressure is discussed.

Keywords: Phase H, dense hydrous magnesium silicates, lower mantle, crystal structure, synthesis