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LETTER

The 10 Å phase: Crystal structure from single-crystal X-ray data

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ABSTRACT

Here we report the results of the first three-dimensional refinement of the 10 Å phase performed with single-crystal X-ray data.

The 10 Å phase, $Mg_3Si_4O_{10}(OH)_2H_2O$, is monoclinic, space group $C2/m$, a = 5.323(1)Å, b = 9.203(1)Å, c = 10.216(1)Å, β = 99.98(1)°, V = 492.9(2) Å^3; the calculated density, assuming Z = 2, is 2.676 g.cm^{-3}. The structure has been solved by direct methods and refined by least-squares method with anisotropic displacement parameters. The final agreement index (R_1) was 0.088 for 54 refined parameters and 499 unique observed reflections collected with a diffractometer with a CCD detector.

The structure of the 10 Å phase is very similar to that of a homo-octahedral, 1 *M* trioctahedral mica: it is a silicate consisting of 2:1 tetrahedral-octahedral layers parallel to (001). The mean Si-O, Mg1-O, and Mg2-O bond lengths are 1.626, 2.082, and 2.081 Å, respectively. The ditrigonal rotation angle α is 0.53°. The interlayer of the 10 Å phase is occupied by water molecules. According to the oxygen occupancy, 1 H_2O p.f.u. is assumed in the investigated sample. Although the average water oxygen position is in the mid-plane, structural refinement suggests disorder along **c***. Twelve hydrogen bonds are located between the water molecule and the 6 + 6 oxygen atoms of the basal rings of adjacent tetrahedral sheets (water-oxygen distances averaging 3.19 Å). Therefore there are six possible orientations for the water molecule, with six hydrogen bonds pointing toward the upper basal ring and six pointing toward the lower ring of tetrahedral sheets. The orientational disorder of water, in agreement with previous Raman spectroscopy data, is a feature relevant to the evaluation of thermodynamic functions and thermal stability of the 10 Å phase, which is a possible water carrier (9.1 wt%) in subducting slabs at high pressure.