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The structure of the 10Å phase from X-ray single crystal diffraction data

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Although the relevance of the 10Å phase as a possible water carrier in subducting slabs at high pressure has been supported by experimental studies (e.g. Fumagalli and Poli, 2004), its crystal structure is not completely known. Previous investigations based on several techniques, i.e. X-ray powder diffraction data, thermal analysis, infra-red and micro-Raman spectroscopy, generally agree with a phlogopite type stacking with T-O-T layers and interlayer molecular water. The amount of extra water that may be hosted in the 10Å phase has been suggested to be variable and depending on synthesis run time (Fumagalli et al., 2001).

We report the results of the first X-ray three-dimensional refinement of the 10Å phase performed on a synthetic high-pressure single-crystal. The 10Å phase 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)$^{\circ}$, V = 492.9(2) Å^3; the calculated density, assuming Z= 2 [Mg_3 Si_4O_{10} $(0H)_2$ $\cdot H_2O$ in the cell], is d_{calc}= 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 on a CCD areal diffractometer.

The structure of the 10Å phase is very similar to that of a homo-octahedral, trioctahedral mica 1M: it is a layer silicate consisting of 2:1 tetrahedral-octahedral layers

parallel to (001). The mean Si – O, Mg(1) - O and Mg(2) - 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 10Å 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****. 12 weak H-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 H-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 in the evaluation of thermodynamic functions and thermal stability of the 10Å phase.

Fumagalli P., Stixrude L., Poli S. and Snyder D. (2001) EPSL, 186, 2, 125-141.

Fumagalli P. and Poli S. (December 3, 2004) Journal of Petrology Advance Access. doi:10.1093/petrology/egh088