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Crystal structure, hydrogen bonding, and high-pressure behavior of the hydroxide perovskite $MgSi(OH)_6$: A phase relevant to deep subduction of hydrated oceanic crust

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Abstract

The structural response to compression of the synthetic high-pressure hydroxide perovskite $MgSi(OH)_6$, the so-called "3.65 Å phase," has been determined to 8.4 GPa at room temperature using single-crystal XRD in the diamond-anvil cell. Two very similar structures have been determined in space groups $P2_1$ and $P2_1/n$, for which differences in oxygen donor-acceptor distances indicate that the non-centrosymmetric structure is likely the correct one. This structure has six nonequivalent H sites, of which two are fully occupied and four are half-occupied. Half-occupied sites are associated with a well-defined crankshaft of hydrogen-bonded donor-acceptor oxygens extending parallel to *c*. Half occupancy of these sites arises from the averaging of two orientations of the crankshaft H atoms ($\| \pm c$) in equal proportions. The $P2_1$ and $P2_1/n$ structures are compared. It is shown that the former is likely the correct space group, which is also consistent with recent spectroscopic studies that recognize six nonequivalent O-H. The structure of $MgSi(OH)_6$ at pressures up to 8.4 GPa was refined in both space groups to see how divergent the two models are. There is a very close correspondence between the responses of the two structures implying that, at least to 8.4 GPa, non-centrosymmetry does not affect compressional behavior. The very different compressional behavior of MgO_6 and SiO_6 octahedra observed in this study suggests that structural phase transformations or discontinuities likely occur in $MgSi(OH)_6$ above 9 GPa.

Keywords: $MgSi(OH)_6$, high pressure, cold subduction, hydrous phase