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Letter

Si-rich Mg-sursassite $Mg_4Al_5Si_7O_{23}(OH)_5$ with octahedrally coordinated Si: A new ultrahigh-pressure hydrous phase

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Abstract

The crystal structure of a new high-pressure hydrous phase, Si-rich Mg-sursassite, of ideal composition $Mg_4Al_5Si_7O_{23}(OH)_5$, that was produced by sub-solidus reaction at 24 GPa and 1400 °C in an experiment using a model sedimentary bulk composition, has been determined by single-crystal X-ray diffraction. The phase was found to be topologically identical to Mg-sursassite, $Mg_5Al_5Si_6O_{21}(OH)_7$, and has space group $P2_1/m$ and lattice parameters a = 8.4222(7), b = 5.5812(3), c = 9.4055(9) Å, β = 106.793(8)°, V = 423.26(6) Å^3, and Z = 1. The empirical formula determined by electron microprobe analysis of the same crystal as was used in the X-ray experiment is $[Mg_{3.93(3)}Fe_{0.03(1)}]_{\Sigma 3.96}[Al_{4.98(3)}Cr_{0.04(1)}]_{\Sigma 5.02}Si_{7.02(4)}O_{23}(OH)_5$, with hydroxyl content implied by the crystal-structure analysis. The most significant aspect of the structure of Si-rich Mg-sursassite is the presence of octahedrally coordinated Si. Its structural formula is $^{M1,VII}Mg_2\ ^{M2,VI}Mg_2^{2+}\ ^{M3,VI}(Al_{0.5}Si_{0.5})_2\ ^{M4,VI}Al_2\ ^{M5,VI}Al_2\ ^{T1,IV}Si_2\ ^{T2,IV}Si_2\ ^{T3,IV}Si_2\ O_{23}(OH)_5$. Si-rich Mg-sursassite joins the group of hydrous ultrahigh-pressure phases with octahedrally coordinated Si that have been discovered by experiment, and that may play a significant role in the distribution and hosting of water in the deep mantle at subduction zones. The reactions defining the stability of Si-rich Mg-sursassite are unknown, but are likely to be fundamentally different from those of Mg-sursassite, and involve other ultrahigh-pressure dense structures such as phase D, rather than phase A.

Keywords: Mg-sursassite, hydrous dense magnesium silicate, synthesis, microprobe analysis, X-ray diffraction, crystal structure