

The crystal structure of $\text{Mg}_8(\text{Mg}_2\text{Al}_2)\text{Al}_8\text{Si}_{12}(\text{O},\text{OH})_{56}$ pumpellyite and its relevance in ultramafic systems at high pressure

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ABSTRACT

Multianvil experiments in the model system $\text{MgO-Al}_2\text{O}_3\text{-SiO}_2\text{-H}_2\text{O}$ at 680 °C and 5.2–6.0 GPa yield a variety of Mg,Al-rich mineral assemblages containing pumpellyite-type phases. Run products include the assemblages pumpellyite-coesite, pumpellyite-forsterite-orthoenstatite and pumpellyite-10 Å phase. The pumpellyite-coesite sample contains pumpellyite with nominal composition $\text{Mg}_8(\text{Mg}_2\text{Al}_2)\text{Al}_8\text{Si}_{12}(\text{O},\text{OH})_{56}$ and about 6 wt% coesite. Powder diffraction data obtained using synchrotron radiation, a parallel-beam Debye geometry, a capillary sample mount, and an Image Plate were refined by Rietveld structure analysis. The structure was modeled in space group $P2_1/m$ [cell $a = 8.5759(4)$, $b = 5.7295(2)$, $c = 18.5376(9)$ Å, $\beta = 97.691(3)^\circ$, $V = 902.66(9)$ Å³] and shows extensive stacking disorder along the [001] direction, which can be described as layers of X-octahedra shifted by (1/2,0,0) vectors. The shifted layers locally show a sursassite-type arrangement. No disorder was detected in the Y-octahedra, which are fully occupied by Al ions, and in the W positions, commonly hosting sevenfold-coordinated Ca atoms in naturally occurring pumpellyite minerals, whereas in the synthetic Mg-rich pumpellyite they are fully occupied by Mg atoms in a distorted sixfold-coordination. The structure can then be described as a pumpellyite-type structure having a certain amount of sursassite domains. Alternative structure models involving: (1) possible presence of ardennite-domains; (2) a sursassite-type structure with pumpellyite domains; (3) cell doubling along c due to long range ordering of the layers containing the X octahedra; or (4) a statistically disordered structure in the centered $A2/m$ parent space group and in other t subgroups, were all tested and discarded on the basis of the full-profile Rietveld refinements of powder diffraction data. The selected model indicates that the polytypic behaviour observed in pumpellyite and related structures (sursassite, and possibly ardennite) is also possible in the high pressure members of the group. The volume of the reaction, MgSiO_3 (enstatite) + 2 Mg_2SiO_4 (forsterite) + $\text{Mg}_8(\text{Mg}_2\text{Al}_2)\text{Al}_8\text{Si}_{12}\text{O}_{42}\text{OH}_{14}$ (pumpellyite) \leftrightarrow 5 $\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$ (pyrope) + 7 H_2O re-evaluated using the new crystallographic data, gave a negative dP/dT slope. The assemblage chlorite-enstatite-pyrope acts as compositional barrier for the occurrence of pumpellyite in most ultramafic compositions for H_2O -undersaturated conditions. In more complex Fe,Ca-containing systems, the preferential partitioning of Fe,Ca in pumpellyite compared to garnet enhances its potential petrological importance in ultramafic subducting slabs.