American Mineralogist, Volume 83, pages 881–888, 1998

Synthesis, crystal structure, and phase relations of $AlSiO_3OH$, a high-pressure hydrous phase

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Abstract

Phase egg, first described by Eggleton et al. (1978), was synthesized and its composition determined to be $AlSiO_3OH$. The crystal structure of $AlSiO_3OH$, including the position of the hydrogen, has been solved and refined from high-resolution X-ray powder diffraction. The resulting lattice constants are $a = 7.14409(2)$ Å, $b = 4.33462(1)$ Å, $c = 6.95253(2)$ Å, and $\beta = 98.396(1)°$. The space group is $P2_1/n$; $Z = 4$, $V_0 = 212.99(1)$ Å^3, and the zero pressure density is 3.74 g/cm^3. This phase, which has features in common with the stishovite structure, occurs above 11 GPa and 700 °C. $AlSiO_3OH$ forms from topaz-OH with increasing pressure and persists to more than 17.7 GPa and 1300 °C. From a Schreinemaker analysis, we predicted that phase egg decomposes with pressure to an unknown, possibly hydrous aluminosilicate. Potentially, phase egg could replace topaz-OH or kyanite in subducted crustal bulk compositions and may transport some water into the deep Earth.