

Crystal structure and compressibility of a two-layer polytype of pseudowollastonite (CaSiO₃)

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ABSTRACT

The crystal structure of a synthetic two-layer polytype of CaSiO₃ pseudowollastonite was determined using single-crystal X-ray diffraction data. It is monoclinic with space group *C2/c* and unit-cell parameters $a = 11.8322(6)$, $b = 6.8624(8)$, $c = 10.5297(5)$ Å, $\beta = 111.245(8)^\circ$, and $V = 796.9(1)$ Å³. The material is isostructural with two-layer SrSiO₃ and SrGeO₃ and has basic structural features similar to those found in four-layer CaSiO₃ pseudowollastonite, except for the stacking sequence of layers of CaO₆ octahedra and Si₃O₉ ternary rings. The compressibility of the structure was measured up to 9.94 GPa and no phase transition was observed. With increasing pressure, all unit-cell parameters decrease nonlinearly with a positive curvature. The axial compression ratios at room pressure are $\beta_a:\beta_b:\beta_c = 2.25:2.36:1.00$ and the bulk modulus, K_T , is 86(1) GPa with $K' = \partial K_T / \partial P = 3.8(4)$.