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Crystal structure and compressibility of a two-layer polytype of pseudowollastonite ($CaSiO_3$)

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ABSTRACT

The crystal structure of a synthetic two-layer polytype of $CaSiO_3$ pseudowollastonite was determined using single-crystal X-ray diffraction data. It is monoclinic with space group *C*2/*c* and unit-cell parameters $a = 11.8322(6)$, $b = 6.8624(8)$, $c = 10.5297(5)$ Å, $\beta = 111.245(8)°$, and $V = 796.9(1)$ Å^3. The material is isostructural with two-layer $SrSiO_3$ and $SrGeO_3$ and has basic structural features similar to those found in four-layer $CaSiO_3$ pseudowollastonite, except for the stacking sequence of layers of CaO_6 octahedra and Si_3O_9 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 $K' = \partial K_T/\partial P = 3.8(4)$.