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On the crystal structure of pseudowollastonite (CaSiO₃)

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ABSTRACT

A single-crystal X-ray diffraction study of synthetic pseudowollastonite (CaSiO₃) shows that this crystal has monoclinic $C2/c$ symmetry, with $a = 6.8394(5)$, $b = 11.8704(9)$, $c = 19.6313(7)$ Å, $\beta = 90.667(6)^\circ$, and $V = 1593.7(2)$ Å³. Basic features of the $C2/c$ structure are similar to those previously determined with a $C\bar{1}$ symmetry but fewer sites exist for the monoclinic space group: five symmetrically nonequivalent Ca sites, three Si sites, and nine O sites.