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Structure of walstromite, $BaCa_2Si_3O_9$, and its relationship to $CaSiO_3$-walstromite and wollastonite-II

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Abstract

The crystal structure of walstromite, ideally $BaCa_2Si_3O_9$, was refined with data from single-crystal X-ray diffraction on a natural specimen from the type locality Esquire No. 8 claim, Big Creek, Fresno County, California, U.S.A. It is triclinic, with space group $P\bar{1}$ and unit-cell parameters $a = 6.7335(2)$, $b = 9.6142(3)$, $c = 6.6859(2)$ Å, $\alpha = 69.638(2)°$, $\beta = 102.281(2)°$, $\gamma = 96.855(2)°$, and $V = 396.01(2)$ Å^3. The only previously published structure for walstromite was based on photographic film intensity data collected from synthetic $BaCa_2Si_3O_9$ (Dent Glasser and Glasser 1968). Due to uncertainty in oxygen positions, the reported final R-factor was 0.16. The current refinement yielded an R-factor of 0.030 with the inclusion of anisotropic displacement parameters.

Walstromite is a Ba-Ca cyclosilicate characterized by Si_3O_9 three-membered rings. It is related to the important calcium silicate group of minerals, especially to $CaSiO_3$-walstromite, through the substitution of Ba into one of the three distinct Ca sites. Joswig et al. (2003) suggested that the structural changes caused by the replacement of Ba^{2+} by Ca^{2+} are minimal and that walstromite is isomorphic with $CaSiO_3$-walstromite, but topologically different from high-pressure wollastonite-II ($Ca_3Si_3O_9$). Our study demonstrates that wollastonite-II and $CaSiO_3$-walstromite are identical phases, and are isostructural with walstromite. This isomorphism implies that the high-pressure $CaSiO_3$ phase may be a potential host for large cations in deep Earth environments.

Keywords: Walstromite, $CaSiO_3$-walstromite, wollastonite-II, crystal structure, single-crystal X-ray diffraction