American Mineralogist, Volume 85, pages 1512–1515, 2000

Rietveld refinement of okayamalite, $Ca_2SiB_2O_7$: Structural evidence for the B/Si ordered distribution

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ABSTRACT

The structure of okayamalite from Arendal, Norway, was refined using the Rietveld method, with Co$K\alpha$ powder X-ray diffraction data (R_F = 3.69%). Okayamalite exhibits a melilite-type structure, space group $P\bar{4}2_1m$, with cell edges a = 7.1248(2), c = 4.8177(2) Å. Si and B are ordered on the T1 and T2 sites respectively, in agreement with the refined tetrahedral distances (<T1-O> = 1.657 Å and <T2-O>= 1.498 Å). In comparison with the other melilite-type compounds, the cation population in okayamalite leads to the minimum structural misfit between tetrahedral and square-antiprism layers.