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The atomic structure of bakerite and its relationship to datolite

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ABSTRACT

Four samples of bakerite, $Ca_4B_5Si_3O_{15}(OH)_5$, were studied by means of IR, TG/DSC, EPMA, and X-ray and neutron diffraction. Chemical analyses can readily discriminate bakerite from datolite, $Ca_4B_4Si_4O_{16}(OH)_4$, by the distinctly lower SiO_2 content of the former. The Rietveld refinement of the combined neutron and X-ray powder data allow the determination of the crystal structure of bakerite to R_p 3.09%. The crystal structure can be derived from that of datolite by the substitution $0.25Si^{4+} + 0.25O^{2-} \leftrightarrow 0.25B^{3+} + 0.25(OH)^-$ at the Si-centered tetrahedral site. This leads to the crystal chemical formula $Ca_4B_5Si_3O_{15}(OH)_5$. Both of the two hydrogen positions in the bakerite structure, one with full occupancy, the other with 25% occupancy, were precisely located. The water molecule generally thought to be present in bakerite structure is actually absent. The excess water detected in chemical analyses can be attributed to the presence of minor impurities. Given the consistent composition of bakerite from various localities and no evidence for substitution of B for Si in datolite, bakerite is retained as a distinct species. A possible explanation of the peculiar 5:3 boron to silicon ratio in bakerite is provided.