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A multi-methodological study of kernite, a mineral commodity of boron

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Abstract

Kernite, ideally $Na_2B_4O_6(OH)_2 \cdot 3H_2O$, is a major constituent of borate deposits and one of the most important mineral commodities of B. The chemical composition and crystal structure of kernite from the Kramer Deposit (Kern County, California) were investigated by a suite of analytical techniques (i.e., titrimetric determination of B content, gravimetric method for Na, ion selective electrode for F, high-*T* mass loss for H_2O content, inductively coupled plasma atomic emission spectroscopy for REE and other minor elements, elemental analysis for C, N, and H contents) and single-crystal X-ray (at 293 K) and neutron (at 20 K) diffraction. The concentrations of more than 50 elements were measured. The general experimental formula of the kernite sample used in this study is $Na_{1.99}B_{3.99}O_6(OH)_2 \cdot 3.01H_2O$. The fraction of other elements is, overall, insignificant: excluding B, kernite from the Kramer Deposit does not act as geochemical trap of other technologically relevant elements (e.g., Li, Be, or REE). The X-ray and neutron structure model obtained in this study confirms that the structure of kernite is built up by: two (crystallographically independent) triangular BO_2OH groups and two tetrahedral BO_4 groups, which share corner-bridging O atoms to form threefold rings, giving chains running along [010], and $NaO_4(OH)(OH_2)$ and $NaO_2(OH)(OH_2)_3$ polyhedra. Positional disorder of two H sites of H_2O molecules was observed by the neutron structure refinement and corroborated by the maximum-entropy method calculation, which consistently provided a model based on a static disorder, rather than a dynamic one. The H-bonding network in the structure of kernite is complex, pervasive, and plays a primary role on its structural stability: the majority of the oxygen sites are involved in H-bonding, as *donors* or as *acceptors*. The potential utilizations of kernite, as a source of B (B_2O_3 ~50 wt%), are discussed, on the basis of the experimental findings of this study.

Keywords: Kernite, borates, mineral commodity, X-ray diffraction, neutron diffraction, crystal chemistry, hydrogen bonding