

## Crystal-chemical reinvestigation of probertite, $\text{CaNa}[\text{B}_5\text{O}_7(\text{OH})_4] \cdot 3\text{H}_2\text{O}$ , a mineral commodity of boron

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### ABSTRACT

The crystal chemistry of probertite, a mineral commodity of B ( $\text{B}_2\text{O}_3 \sim 50$  wt%) with ideal formula  $\text{CaNa}[\text{B}_5\text{O}_7(\text{OH})_4] \cdot 3\text{H}_2\text{O}$  from the Kramer Deposit (Kern County, California, type locality), was investigated by a multi-methodological approach [i.e., single-crystal X-ray (at 293 K) and neutron (at 20 K) diffraction, EPMA-WDS, LA-ICP-MS, and LA-MC-ICP-MS]. As recently determined for other hydrous borates, the real chemical formula of probertite from the Kramer Deposit is virtually ideal, i.e., the fractions of other elements are insignificant. Therefore, excluding B, probertite does not act as a geochemical trap of other industrially relevant elements (e.g., Li, Be, or REE). Our experimental results confirm that the structure of probertite is built up by the so-called pentaborate polyanion  $[\text{B}_5\text{O}_7(\text{OH})_4]^{3-}$  (topology:  $5(2\Delta + 3T)$ ), which consists of oxygen-sharing B-tetrahedra and B-triangular units. The five (geometrical) components of the polyanion are  $\text{BO}_3$ ,  $\text{BO}_2\text{OH}$ ,  $\text{BO}_4$ ,  $\text{BO}_3\text{OH}$ , and  $\text{BO}_2(\text{OH})_2$  groups. The pentaborate building units are connected to form chains running along  $[100]$ . Clusters of distorted Ca-polyhedra  $[\text{CaO}_5(\text{OH})_3(\text{OH}_2)]$ , CN = 9] and Na-polyhedra  $[\text{NaO}(\text{OH})_2(\text{OH}_2)_3]$ , CN = 6] are mutually connected by edge-sharing and, in turn, connected to the pentaborate chains by edge-sharing (with the Ca-polyhedron) and corner-sharing (with the Na-polyhedron). The hydrogen-bonding scheme of the probertite structure is complex and pervasive, with 10 independent H sites (belonging to hydroxyl groups or  $\text{H}_2\text{O}$  molecules) and 11 of the 14 oxygen sites being involved in H-bonds as donor or acceptors. Hence, the H-bonding network likely plays an important role in the stability of probertite. In addition, the potential utilizations of probertite are discussed.

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