A multi-methodological study of kurnakovite: A potential B-rich aggregate

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ABSTRACT

The crystal structure and crystal chemistry of kurnakovite from Kramer Deposit (Kern County, California), ideally MgB₆O₁₀(OH)₄·5H₂O, were investigated by single-crystal neutron diffraction (data collected at 293 and 20 K) and by a series of analytical techniques aimed to determine its chemical composition. The concentration of more than 50 elements was measured. The empirical formula of the sample used in this study is Mg₀.₉₂(Si₀.₉₁B₃.₀₂O₃.₀₁)(OH)₄·4.₉₈H₂O. The fraction of rare earth elements (REE) and other minor elements are, overall, insignificant. Even the content of fluorine, as a potential OH-group substituent, is insignificant (i.e., ~0.008 wt%). The neutron structure model obtained in this study, based on intensity data collected at 293 and 20 K, shows that the structure of kurnakovite contains: [BO₃(OH)]-groups in planar-triangular coordination (with the B-ions in sp² electronic configuration), [BO₃(OH)₂]-groups in tetrahedral coordination (with the B-ions in sp³ electronic configuration), and Mg(OH)₂(H₂O)₂-octahedra, connected into (neutral) Mg₃(H₂O)₈O₂(OH)₄ units forming infinite chains running along [001]. Chains are mutually connected to give the tri-dimensional structure only via hydrogen bonding, and extra-chains “zeolitic” H₂O molecules are also involved as “bridging molecules.” All the oxygen sites in the structure of kurnakovite are involved in hydrogen bonding, as donors or as acceptors.

The principal implications of these results are: (1) kurnakovite does not act as a geochemical trap of industrially relevant elements (e.g., Li, Be, or REE), (2) the almost ideal composition makes kurnakovite a potentially good B-rich aggregate in concretes (for example, used for the production of radiation-shielding materials for the elevated ability of 10B to absorb thermal neutrons), which avoids the risk to release undesirable elements, for example sodium, that could promote deleterious reactions for the durability of cements.

Keywords: Kurnakovite, borates, single-crystal neutron diffraction, crystal chemistry, hydrogen bonding, B-rich aggregate

INTRODUCTION

Kurnakovite, with the ideal chemical formula MgB₆O₁₀(OH)₄·5H₂O, is a complex hydrous borate mineral found as a common constituent of borate deposits, along with borax [ideally Na₂(B₂O₃)(OH)₄·8H₂O] and ulexite {ideally NaCa[B₂O₃(OH)₂]·5H₂O}. Natural borates represent the most important source of boron, which is an important geochemical marker for petrogenetic processes (especially in pegmatitic and granitic systems) and a strategic element for technological materials (e.g., to lower melting temperatures and melt viscosities in silicate glass systems), but they are also being used for the production of radiation-shielding materials for the elevated ability of ¹⁰B to absorb thermal neutrons. More specifically, the most important use is to absorb neutrons emitted by nuclear reactors for energy production, scientific research, or medical applications, which promotes the development of suitable materials able to shield from harmful radiations. Approximately 20% of natural boron is ¹⁰B, which shows a high capacity to absorb thermal neutrons due to its high cross section for the ¹⁰B(n,α)Li reaction (~3840 barns; Carter et al. 1953; Palmer and Swihart 1996; Rauch and Waschkowski 2002). Borax and ulexite have been objects of investigation to produce B-rich aggregates in concretes. However, these two minerals have proved they induce a drastic effect on setting and hardening, coupled with a drastic lowering of strength development and durability of concretes (e.g., Glinicki et al. 2018). In addition, these minerals dissolve into the paste, releasing sodium, that could potentially promote deleterious reactions for the durability of Portland cements. On the other hand, the use of the most stable compounds, for example like the synthetic B₃C or B-mullites, is not environmentally and economically sustainable (Okuno et al. 2009; Gatta et al. 2013; Di Julio et al. 2017). In the framework of a long-term project to select new potential substitutes of borax and ulexite as B-bearing aggregates, using a multi-methodological approach we have

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