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

G. Diego Gatta[1,*], Alessandro Guastoni[2], Paolo Lotti[1], Giorgio Guastella[3], Oscar Fabelo[4], and Maria Teresa Fernandez-Diaz[4]

[1]Dipartimento di Scienze della Terra, Università degli Studi di Milano, Via Botticelli 23, I-20133 Milano, Italy. Orcid 0000-0001-8348-7181
[2]Dipartimento di Geoscienze, Università degli Studi di Padova, Via G. Gradenigo 6, I-35131, Padova, Italy
[3]Agenzia delle Dogane e dei Monopoli, Direzione Regionale per la Lombardia, Laboratorio e Servizi Chimici, Via Marco Bruto 14, I-20138 Milan, Italy
[4]Institut Laue-Langevin, 71 Avenue des Martyrs, F-38000 Grenoble, France

Abstract

The crystal structure and crystal chemistry of kurnakovite from Kramer Deposit (Kern County, California), ideally $MgB_3O_3(OH)_5 \cdot 5H_2O$, 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 $Mg_{0.99}(Si_{0.01}B_{3.00})_{\Sigma 3.01}O_{3.00}(OH)_5 \cdot 4.98H_2O$. 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: $[BO_2(OH)]$-groups in planar-triangular coordination (with the B-ions in sp^2 electronic configuration), $[BO_2(OH)_2]$-groups in tetrahedral coordination (with the B-ions in sp^3 electronic configuration), and $Mg(OH)_2(H_2O)_4$-octahedra, connected into (neutral) $Mg(H_2O)_4B_3O_3(OH)_5$ 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" H_2O 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 ^{10}B 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