



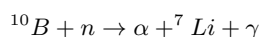
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## Thermal and compressional behavior of the natural borate kurnakovite, (MgB<sub>3</sub>O<sub>3</sub>(OH)·5H<sub>2</sub>O)

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Natural borates are minerals of relevant economic interest, as they represent the main source of boron (i.e. since 2014, in the Critical Raw Material list for the Europe's economy). The peculiar properties of boron opened several routes of applications in a large variety of industrial sectors, including glass, ceramics, electronics, metallurgy, textile, cosmetics and chemistry [1]. Moreover, boron also finds applications as a fundamental constituent of neutron radiation-shielding materials, which are used in nuclear energy plants, as well as in facilities for scientific research or medical applications [2]. The high capability of borates to act as neutron-shielding materials is due to the isotope <sup>10</sup>B, representing about 20% of natural boron, having a high cross section (~ 3840 barns) for thermal neutrons, leading to the following reactions:



In this light, kurnakovite (MgB<sub>3</sub>O<sub>3</sub>(OH)·5H<sub>2</sub>O,  $a = 8.308(7)$   $b = 10.599(2)$   $c = 6.442(3)$   $\alpha = 98.85(3)$   $\beta = 109.09(6)$   $\gamma = 105.57(4)$ , space group =  $P\bar{1}$ ) was selected as a promising natural candidate in neutron radiation-shielding materials, based on Portland or Sorel cements [3]. Moreover, the absence of Na prevents the occurrence of alkali-silica reactions, which can decrease the durability and the mechanical strength of Portland cements [4]. In this study, the thermal and compressional behaviour of kurnakovite was investigated (up to 13.65(5) GPa and in a T range 100(2) – 393(2) K) by means *in-situ* single-crystal synchrotron X-ray diffraction experiments, performed at the XRD1 beamline at Elettra (Trieste, Italy) and at P2.02 beamline at PETRA-III (Hamburg, Germany). The bulk thermal expansion coefficient was calculated based on the non-ambient T data, yielding to the value of  $\alpha_V = 5.18(1) \cdot 10^{-5} \text{K}^{-1}$ . The crystal structure showed the first evidence of collapse at  $T > 393$  K and completely amorphized at 423 K, posing questions on the potential application as matrix-aggregates in radiation-shielding concretes [4]. The refined bulk modulus of kurnakovite resulted to be  $K_{V0} = 35(3) \text{GPa}$ . A reconstructive phase transition was observed in the range 9.23(5) – 11.11(5) GPa [4]. The high-P polymorph, kurnakovite-II, is still triclinic with a unit cell volume three times larger with respect to kurnakovite [4]. As observed in other borates (e.g. ulexite and colemanite [5,6]), only a fraction of trigonal-planar B increases its coordination to tetrahedral by bonding with a H<sub>2</sub>O-oxygen atom [4].

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