ID15b and Hydrated borates at High-pressure

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Abstract

Hydrated borates, such as colemanite, kernite, ulexite, and borax, represent the primary ore minerals of boron—a critical geochemical marker for petrogenetic processes and a strategic resource for advanced technological applications. Classified as critical raw materials by the EU in 2017[1], these minerals are increasingly investigated as aggregates in neutron-shielding concretes due to their high thermal neutron absorption capacity, stemming from their elevated H and ^{10}B content. Structurally, hydrated borates consist of $B\varphi_x$ units (tetrahedra and trigonal planes), where φ represents an oxygen atom or a OH^- group or a H_2O molecule, organized into polyion clusters, which are linked to alkali or alkaline-earth polyhedra (*e.g.*, Na^+, $Ca2^+$, Mg^{2+}). Within these frameworks, H_2O molecules and OH^- groups form an extensive hydrogen-bond network that is fundamental to the stability of the crystalline edifice [2, 3]. This contribution explores the high-pressure deformation mechanisms and structural evolution of various hydrated borates, investigated via synchrotron X-ray diffraction at the ID15b beamline (ESRF). Our results show that these minerals undergo several high-pressure phase transitions. These involve the conversion of trigonal $B\varphi_3$ units into $B\varphi_4$ tetrahedra through the formation of additional B-φ bonds, or the rearrangement of the coordination spheres surrounding the divalent/trivalent cations (*e.g.*, Fig. 1). Interestingly, a recurrent structural pattern appears to emerge, potentially providing a basis for a predictive framework regarding the high-pressure stability of this mineral class (Fig. 2).

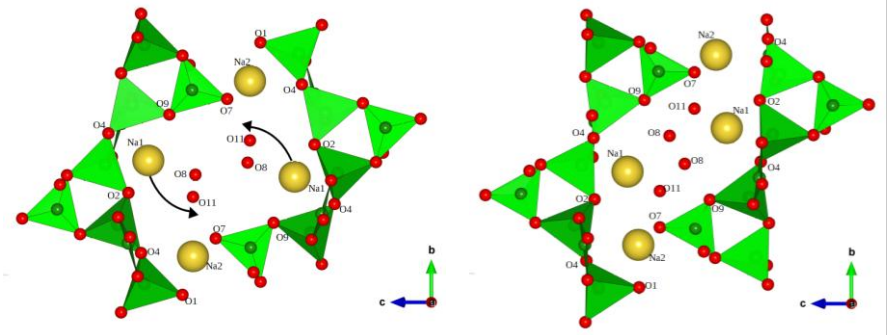

Fig.1: difference between the structures of kernite (left) and kernite-II (right)

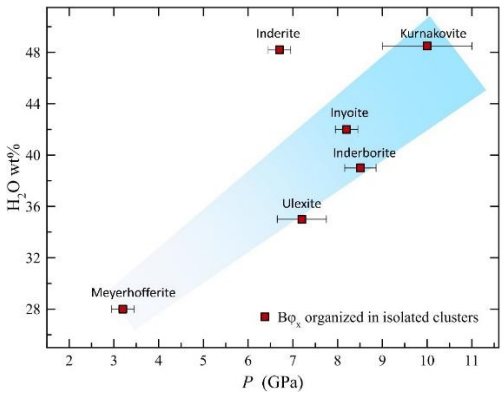

Fig.2: H_2O wt% *vs* $P_{(phase\ transition)}$ in a number of hydrated borate structures

References

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[3] Comboni D., Battiston T., Lotti P., Hanfland M., Gatta G.D. (2024) Atomic-scale deformation mechanisms at high-pressure in inderborite, $CaMg[B_3O_3(OH)_5]2(H_2O)_4{\cdot}2H_2O$. Mineralogical Magazine, 88, 473–481 https://doi.org/10.1180/mgm.2024.29.