Poster

Structural evolution and pressure-driven phase transitions in hydrated borates

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Hydrated borates (*e.g.*, borax, tincalconite, colemanite, kernite, ulexite) are the most common ore minerals of boron, an important geochemical marker, in pegmatitic and granitic systems, for petrogenetic processes and a strategic element in a series of technological applications. Hydrated borates have been listed as critical raw materials by the EU [1], and they could be used as aggregate in neutronshielding Sorel or Portland concretes, enhancing the adsorption of concrete towards thermal neutrons. The main structural units in hydrated borates are B φ_x units (fundamental building blocks, *i.e.*, tetrahedra and planar trigonal group where φ is an anion, O²⁻ or OH⁻), connected in such a way to form clusters of polyions connected to alkaline/Earth alkaline (mainly Na⁺, K⁺, Ca²⁺, Mg²⁺) polyhedra. In these structures, H₂O molecules and OH⁻ form a complex and pervasive hydrogen-bond network, which reinforce the connection between the polyions clusters and the cations-polyhedrons, playing a paramount role in the stability of the crystalline edifice [2, 3]. In the last 4 years, a number of studies have been performed at high pressure unveiling phase transition driving deformation mechanisms' that lead to the formation of their high-pressure polymorphs (Fig. 1). Critically, the pressure at which hydrated borates undergo a phase transition is related to the water content of the mineral itself. The aim of this contribution is to provide insides on the high-pressure behavior and structure evolution of selected hydrate borate minerals.



Figure 1. Water content *vs* pressure at which hydrated borates undergo a phase transition (* paper under review, [§]data collected and still unpublished). FBBs: fundamental building blocks.

- [1] EU Commission, Study on the review of the list of critical raw materials, 2017.https://doi.org/10.2873/876644.
- [2] Pagliaro, F., Lotti, P., Battiston, T., Comboni, D., Gatta, G.D., Cámara, F., Milani, S., Merlini, M., Glazyrin, K., Liermann, H. (2021) Constr. Build. Mater., 266, 121094.
- [3] Comboni, D., Poreba, T., Pagliaro, F., Battiston, T., Lotti, P., Gatta, G.D., Garbarino, G., Hanfland, M. (2021). Acta Crystallogr. B., 6, 940-945.