

Phase stability of hydrated borates at high pressure

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Hydrated borates are a class of minerals made by clusters or chains of $B\phi_x$ groups (ϕ represents an oxygen, an H_2O molecule or an OH) organized either in tetrahedra or in planar trigonal groups. Hydrated borates are believed to be a cheaper alternative to B_4C for radiation-shielding concretes (Okuno et al., 2005), due to the large cross section (~ 3840 barns) for thermal neutrons of the isotope ^{10}B , which represents about 20% of the boron in nature. A comprehensive characterization of the crystal-chemistry, elastic properties, stability and structural behavior of natural borates at varying T and P conditions is advisable for modelling and understanding their role when utilized as aggregates in radiation-shielding concretes (Torrenti et al., 2010), in which the components are subject to pressure (by static compression) and temperature (by irradiation). Interestingly, all hydrated borates studied so far at high-pressure display one (or more) phase transition, and the pressure at which the phase transitions occur seems to be correlated to the H_2O content of the minerals (e.g., Comboni et al., 2020, 2021). During the phase transitions, the most dramatic structural change is the increase of the coordination number of part of the ^{III}B to ^{IV}B , by the interaction between the ^{III}B and one H_2O molecule or OH group, underlying the importance of the hydrogen bond network in the stability of the crystalline structure.

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