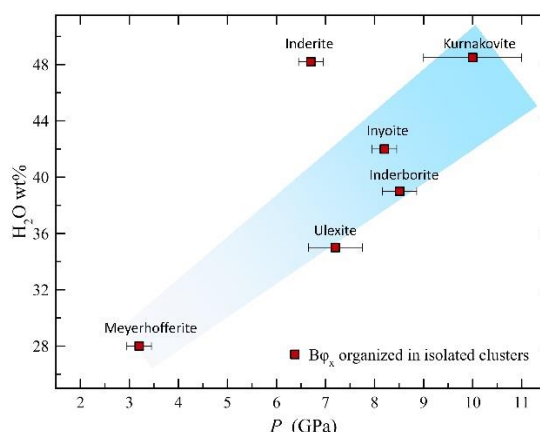


# Phase transitions and crystal structure evolution of hydrated borates at non-ambient conditions

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Hydrated borates are a class of minerals composed of clusters or chains of  $B\phi_x$  groups (where  $\phi$  represents an oxygen atom, a  $H_2O$  molecule, or an  $OH^-$  group) organized either in tetrahedra or planar triangular groups. Hydrated borates are considered a more cost-effective alternative to  $B_4C$  in radiation-shielding concretes [1], primarily due to the significant cross-section ( $\sim 3840$  barns) for thermal neutrons of the  $^{10}B$  isotope, which represents approximately 20% of natural boron. It is advisable to comprehensively characterize the crystal chemistry, elastic properties,  $P$ - $T$  phase stability fields, and structural behaviour of natural borates under varying temperature and pressure conditions to model and understand their role as aggregates in radiation-shielding concretes [2], where the components experience pressure (*via* static compression) and temperature (*via* irradiation). Since 2018, my research group has conducted an extensive study of economically valuable hydrated borates, as well as common complementary phases occurring in borates deposits. High-pressure investigations of all studied hydrated borates have revealed one or more phase transitions occurring at pressures below 11 GPa, and the occurrence of these transitions appears to be highly correlated with the  $H_2O$  content of the minerals (*e.g.*, [3-4]). In response to the phase transitions, the most significant structural change observed in our experiments is the increase in the coordination number of alkali/alkaline-earth cations as well as of part of the boron population, from  $^{III}B$  to  $^{IV}B$ , due to the interaction between  $^{III}B$  and  $H_2O$  molecules. This, on the other hand, emphasizes the importance of the hydrogen bond network, usually with complex and pervasive configuration, in preserving the stability of the crystalline edifice of this class of materials.



**Fig. 1:**  $H_2O$  content vs. pressure at which the phase transition occurs in borate structures characterized by isolated polyions. A qualitative linear correlation is represented by the sky-blue shade

## References

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