

High-pressure phase transition and crystal structure evolution of inderite,



Comboni D. ^{* 1}, Battiston T. ¹, Lotti P. ¹, Gatta G. D. ¹

¹Earth Science Department, University of Milan, Italy

*Presenting author; E-mail: davide.comboni@unimi.it

Abstract text

Inderite, ideally $[\text{MgB}_3\text{O}_3(\text{OH})_5 \cdot 5\text{H}_2\text{O}]$, is a light (1.80 g/cm^3) Na-free hydrated borate, discovered in the Inder deposit (Kazakhstan), which could be efficiently employed in radiation-shielding concretes due to its relatively high B_2O_3 content ($\sim 37 \text{ wt}\%$). The crystal structure of inderite is made by $[\text{B}_3\text{O}_3(\text{OH})_5]^{2-}$ polyions, organized in 3-membered rings of 2 $\text{B}\phi_4$ tetrahedra and one $\text{B}\phi_3$ unit (where ϕ is an anion; O^{2-} or OH). Prior to any utilization, is advisable to correctly characterized the thermodynamic parameters of any aggregate, if used in neutron-shielding concretes, where temperature can increase due to the interactions with the highly energetic neutron beam. Overall, phase transitions occurring at different pressures (and temperatures) were discovered in all the hydrous borates investigated so far (*e.g.*, [1, 2]), suggesting that the high-pressure stability of hydrated borates having polyions organized in isolated units (*e.g.*, inderite) is directly correlated with the total H_2O content of the mineral itself. Inderite is the ideal case-scenario to validate this model and here we report the results of this study that leads to: 1) track the isothermal compressional path, based on the experimental P - V data, 2) derive the elastic parameters, currently unavailable in the literature; 3) investigate the phase-stability field of inderite at *high-pressure*; 4) describe the *high-pressure* structural re-arrangement of inderite at the atomic scale.

References

- [1] Pagliaro F., Lotti P., Battiston T., Comboni D., Gatta G.D., Cámara F., Milani S., Merlini M., Glazyrin K., Liermann H. (2021) Thermal and compressional behavior of the natural borate kurnakovite, $\text{MgB}_3\text{O}_3(\text{OH})_5 \cdot 5\text{H}_2\text{O}$. *Construction and building materials*, 266, 121094.
- [2] Comboni D., Poreba T., Pagliaro F., Battiston T., Lotti P., Gatta G.D., Garbarino G., Hanfland M. (2021) Crystal structure of the high-P polymorph of $\text{Ca}_2\text{B}_6\text{O}_6(\text{OH})_{10} \cdot 2(\text{H}_2\text{O})$ (meyerhofferite). *Acta Crystallographic Section B*, 6, 940-945.