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# Association Française de Cristallographie

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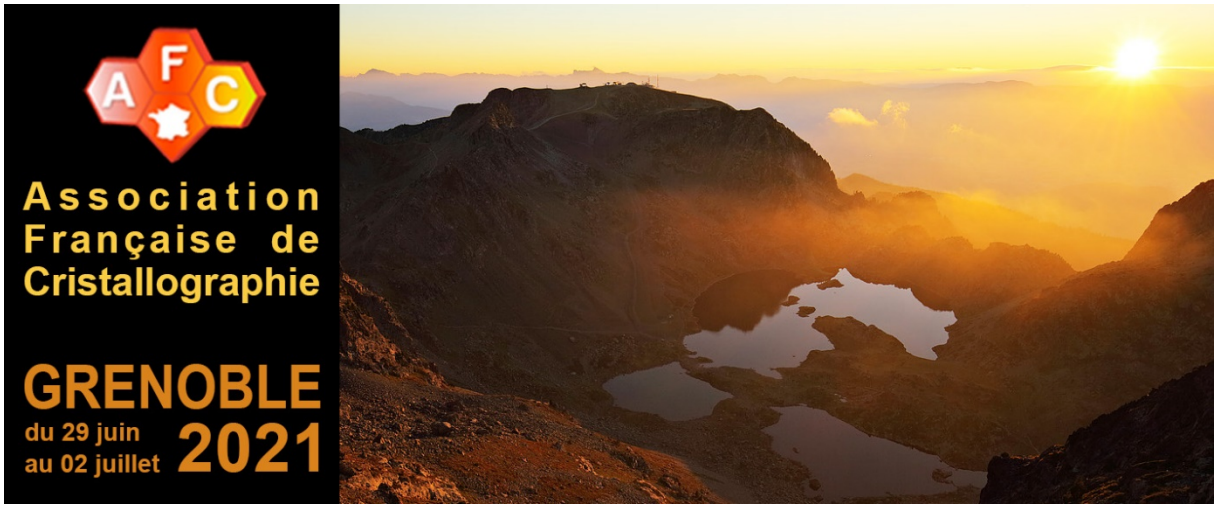

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# High-pressure behaviour and phase transition of ulexite at ID15b (ESRF)

Poster

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Ulexite (ideally, $NaCaB_5O_6(OH)_6 \cdot 5(H_2O)$, a ~8.816 Å, b ~12.87 Å, c ~6.678 Å, α~90.4°, β~109.1°, γ~105.0°, Sp. Gr. P-1 ), is one of the most common borates and, alongside with kernite, borax and colemanite, accounts roughly for 90% of the borates used worldwide [1]. Borates and boron-based materials are widely used in a number of products such as heat-resistant pyrex, low-thermal expansion glasses, laundry bleaches and detergents etc. [e.g., 2]. Notably, ulexite and other borates with a high content of $B_2O_3$, having relatively low cost and good abundance in nature (e.g., kernite, colemanite), are currently studied to assess their utilization as light aggregates in radiation-shielding materials due to the isotope $^{10}B$ (accounting for about 20 % of natural boron) high cross section for thermal neutrons (~3840 barns) [3]. Therefore, enhanced neutron radiation shielding capacity of protective structures can be achieved using cement-based composites with boron-containing aggregates [4]. Therefore, ulexite could be used for the production of concretes and a few studies have been devoted to determine the role of ulexite on the mortars and concretes properties. However, a full and comprehensive characterization of the elastic parameters, phase-stability and structural behavior at the atomic scale at varying *T* and *P* conditions, is still missing. Such information would be critical to model its thermo-mechanical properties when used as an aggregate, especially in neutron-shielding concretes. For this reason, the high-pressure behavior of ulexite has been investigated by *in-situ* single-crystal X-ray diffraction under hydrostatic conditions. Analysing the pressure-volume data and the diffraction patterns, we were able to: 1) model the *P-V* data and calculate the compressibility parameters; 2) investigate the phase-stability field of ulexite at high pressure; 3) resolve the structure of the high-pressure polymorph of ulexite.

**Références**

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