

## **Pressure-induced over-hydration of thomsonite: A synchrotron powder diffraction study**

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### **ABSTRACT**

The structural behavior of thomsonite compressed in aqueous medium up to 3 GPa was studied by means of in situ synchrotron powder diffraction with a diamond anvil cell. In the range between 0.0001 and 2 GPa, the compressibility of thomsonite is markedly lower than that reported previously, where a non-penetrating medium (with only 6% H<sub>2</sub>O) was used. This indicates a pressure-induced hydration (PIH), which results in the transition to an over-hydrated phase observed at 2 GPa. The structure of over-hydrated thomsonite contains one additional, half-occupied H<sub>2</sub>O position, coordinated by the calcium at the Ca2 site, with a scolecite-like coordination [CaO<sub>4</sub>(H<sub>2</sub>O)<sub>3</sub>]. The appearance of new H<sub>2</sub>O position causes a 4.5% volume expansion through the cooperative rotation of [T<sub>2</sub>O<sub>5</sub>]<sup>∞</sup> chains, leading to the enlargement of the cross-section of the main channels parallel to *c* axis. The observed deformation mechanism is similar to that found in high-hydrated and super-hydrated natrolite, although only a half of the channels are affected by PIH. The present data indicate that the over-hydration effect in fibrous zeolites strongly depends on the partial water pressure in compressing medium.

**Keywords:** Zeolite, thomsonite, high pressure, compressibility, phase transition, crystal structure, over-hydration