

Elastic behavior of zeolite boggsite in silicon oil and aqueous medium: A case of high-pressure-induced over-hydration

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ABSTRACT

This paper reports the results of an in situ high-pressure synchrotron X-ray powder diffraction investigation on the natural zeolite boggsite $[(K_{0.06}Na_{0.36}Sr_{0.01}Ca_{7.00}Mg_{1.20})(Al_{17.52}Si_{78.62}Fe_{0.05}O_{192}) \cdot 82.3 H_2O]$. The study was performed using both a (16:3:1) methanol:ethanol:water mixture (m.e.w.) as a nominally “penetrating” hydrostatic *P*-transmitting medium and silicon oil (s.o.) as a “non-penetrating” medium. The studied pressure ranges are: P_{amb} –7.6 and P_{amb} –5.9 GPa in m.e.w. and s.o., respectively. No complete X-ray amorphization is observed up to the highest investigated pressures, and the original unit-cell parameters are almost completely recovered upon decompression in both media. The reductions of *a*, *b*, *c*, and *V*, within the pressure-ranges investigated, are 5.3, 4.2, 4.0, and 13.0% in s.o. and 4.1, 4.1, 3.8, and 11.5% in m.e.w. The Rietveld structural refinements of the powder patterns of the experiments in m.e.w. converged successfully up to 3.6 GPa and demonstrated the penetration of 13 additional water molecules between 0.3 and 2.9 GPa. This over-hydration occurs without any unit-cell volume expansion and can be explained by the fact that no new extraframework sites arise during compression and that water penetration is the only factor to increase the occupancy of already existing sites. Boggsite compressibility is higher in s.o. than in m.e.w. In particular, compressibility in m.e.w. is lower below 3 GPa, whereas above this pressure, the *P*-*V* trend becomes similar in the two media. This can be ascribed to the fact that, during water molecule penetration ($0.3 < P < 3$ GPa), the effect of the *P*-transmitting medium is directed to compress the system as well as to penetrate the channels.

Keywords: Zeolite, boggsite, high pressure, compressibility, over-hydration, crystal structure, synchrotron XRPD data