

Hydrogen-bond system and dehydration behavior of the natural zeolite parthéite

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ABSTRACT

The crystal structure, including H positions, of the monoclinic zeolite mineral parthéite (space group *C2/c*) of framework type **-PAR** from Denezhkin Kamen (Urals, Russia) was refined, from single-crystal X-ray data to $R_1 = 3.46\%$. In addition, in situ single-crystal X-ray data have been measured in steps of 25 °C up to 375 °C to analyze dehydration behavior. In situ Raman spectra of the natural (room temperature) and partly dehydrated varieties of parthéite have been recorded at 100, 150, and 275 °C.

The structure of parthéite, $\text{Ca}_2\text{Al}_4\text{Si}_4\text{O}_{15}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$, is characterized by a tetrahedral framework interrupted by an OH-group forming the apex of one AlO_4 tetrahedron. In addition, this OH-group coordinates extraframework Ca together with two H_2O molecules and four framework oxygen sites. The structure has four strong hydrogen bonds with $\text{H} \cdots \text{O}$ interactions below 2 Å. The fifth hydrogen associated with a H_2O molecule, exhibits two potential acceptors of weak hydrogen bonds with $\text{H} \cdots \text{O}$ distances of ca. 2.5 Å. This softly bound H_2O molecule is released at 150 °C without severe impact on framework distortions but with decrease of Ca coordination from seven to six. Concurrently with loss of the second H_2O molecule at 250 °C, the structure further compacts and becomes severely distorted. The space group *C2/c* and the tetrahedral connectivity are preserved but β changes from 91 to 79° and the volume drops from 1730 to 1600 Å³. Ca is still six-coordinated by five framework O atoms and OH.

Keywords: Zeolite, parthéite, hydrogen bonding, dehydration, Raman spectroscopy, crystal structure