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

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The crystal structure, including H positions, of the monoclinic zeolite mineral parthéite $Ca_2Al_4Si_4O_{15}(OH)_2 \times 4H_2O$ of framework type -PAR from Denezhkin Kamen (Urals, Russia) was refined from single crystal X-ray data (C2/c, a = 21.5474(4)Å b = 8.75638(15)Å c = 9.30578(16)Å β = 91.5524(18)°). In addition, in situ high-temperature single-crystal X-ray data have been measured in steps of 25 °C up to 375 °C to analyse dehydration behaviour. 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 (Engel and Yvon 1984) is characterized by complete order of tetrahedral Si and Al and oblate ten-membered ring channels running parallel to the c axis. The apex of one AlO4 tetrahedron is terminated by an OH group. Pockets within the channels host extraframework Ca coordinated by four framework oxygens, one OH-group and two H_2O molecules. The structure has four strong hydrogen bonds with H...O interactions below 2 Å. The fifth hydrogen associated with a H_2O molecule, exhibits two potential acceptors of weak hydrogen bonds with H...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 changed from 91° to 101° and the volume dropped from 1730 to 1600 Å3. Ca is still six-coordinate by five framework oxygens and OH. The interrupted tetrahedral framework with a terminate OH group linked to an Al tetrahedron has special flexibility (up to 400 °C) enabling to accomplish six-fold Ca coordination even if all H_2O molecules are expelled.

Engel, N. and Yvon, K. (1984) The crystal structure of parthéite. Zeitschrift für Kristallographie, 169, 165-175.