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Crystal structure of dehydrated ulexite, $NaCaB_5O_6(OH)_6 \cdot 3H_2O$

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Abstract

Ulexite, a key borate mineral exploited in various industrial applications, undergoes thermal transformations. Here, we report the determination of the crystal structure of dehydrated ulexite, $NaCaB_5O_6(OH)_6 \cdot 3H_2O$, for the first time, using the single-crystal X-ray diffraction technique. Thermal analysis and synchrotron powder diffraction reveal that ulexite, $NaCaB_5O_6(OH)_6 \cdot 5H_2O$, loses two H_2O molecules at 100 °C, causing the formation of a stable three-hydrated phase that retains the fundamental building block (FBB) observed in ulexite. The dehydrated ulexite is triclinic with space group $P\bar{1}$ and lattice parameters $a = 8.686(4)$ Å, $b = 10.973(5)$ Å, $c = 6.709(3)$ Å, $\alpha = 105.463(5)°$, $\beta = 107.518(5)°$, $\gamma = 79.833(5)°$, and $V = 584.5(5)$ Å^3. A distinctive rearrangement of the Na coordination environment from the original six- to seven-coordinated geometry is observed, whereas the Ca atom retains an eight-coordinated geometry. The Na-O and Ca-O bond distances range from 2.340 to 2.852 Å and 2.379 to 2.646 Å, respectively. These polyhedra form edge-sharing chains that interconnect in two-dimensional sheets on the *b*-*c* plane. The FBB of the dehydrated ulexite comprises double three-membered rings consisting of a central BO_4 tetrahedron, a $BO_2(OH)_2$ tetrahedron, and $BO_2(OH)$ triangle sharing corners, described as $2\Delta 3\square$: $<\Delta 2_\square>-<\Delta 2_\square>$. The average B-O bond distances of two $B\varphi_3$ triangles (φ: O or OH) are 1.363 and 1.368 Å, whereas those of three $B\varphi_4$ tetrahedra are 1.475, 1.477, and 1.474 Å. The dehydrated ulexite is stable up to 160 °C. Our findings not only resolve longstanding ambiguities regarding the nature of the so-called one-hydrated phase but also suggest the possibility that dehydrated ulexite naturally emerges as a stable hydrated borate mineral. New insights into the thermal behaviors and dehydration mechanisms of hydrated borate minerals have implications for both natural mineralization processes and industrial applications.

Keywords: Ulexite, dehydration, thermal transformation, dehydrated ulexite, single-crystal X-ray diffraction