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Dehydration and rehydration processes in gmelinite: An in situ X-ray single-crystal study

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Abstract

The dehydration-rehydration process in gmelinite-Na $|Na_{7.27}K_{0.28}Ca_{0.15}(H_2O)_{21.85}|[Al_{7.71}Si_{17.24}O_{48}]$-GME, a natural zeolite that can be described as a parallel stacking of double six rings of tetrahedra in the AABB sequence, was studied by X-ray diffraction data. Its space group is $P6_3/mmc$ with a = 13.764(1) and c = 10.078(1) Å cell parameters. Single-crystal data collections were performed at room conditions and at increasing temperatures, in a hot nitrogen stream, up to the fragmentation of the crystals, which occurs at a temperature as low as 100 °C, and afterward the crystal was cooled down to room conditions. X-ray powder diffraction data showed that gmelinite-Na transforms into a new structure with an AFI-type topology at about 300 °C. At room conditions, extraframework cations are located in two symmetrically independent positions, both of which are coordinated to either framework O atoms or water molecules. When the mineral is heated to 90 °C, about 40% of H_2O is lost, and one cation site splits over two positions, which are three-coordinated to the framework O atoms. The dehydration process is completely reversible over a period of hours. X-ray single-crystal data has highlighted that gmelinite-Na when quenched at 100 K displays remarkable modifications in its extraframework content, resulting in a strong disorder in its extraframework ions. As in the case of heating, the mineral restores its structural features when brought back to room temperature.

Keywords: Gmelinite, dehydration, rehydration, in situ crystal structure, low temperature