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Stepwise dehydration of Sr-exchanged heulandite: A single-crystal X-ray study

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ABSTRACT

A Sr-exchanged heulandite crystal of composition $Sr_{4.35}Ca_{0.13}(Al_{8.96}Si_{27.04}O_{72})\cdot 26H_2O$ was used for stepwise dehydration experiments. The crystal was heated for approximately 12 h from room temperature to 250 °C in steps of 50 °C using an airflow-heater device. For single-crystal X-ray data collection the crystal was quenched to –173 °C with liquid-N_2 on the diffractometer. Due to pronounced Sr order deviating from the topological symmetry *C*2/*m*, the structure was refined in space group *Cm* for each dehydration state. The initial H_2O content of 26 molecules per formula unit (pfu) at room temperature decreased to 17 molecules pfu after heating at 250 °C. Heating to 270 °C mechanically destroyed the crystal and a completely dehydrated state could not be studied. The loss of H_2O and accompanying migration of Sr caused a change of cell parameters: *a* and *c* slightly decreased, *b* decreased, and β remained invariant, leading to a reduction of the cell volume. As Sr loses H_2O upon dehydration, it moves toward the C rings and forms stronger bonds to the tetrahedral framework. With increasing dehydration the A and B ring become slightly compressed and elongated. Initially highly populated Sr sites split into less populated sites caused by the loss of surrounding H_2O molecules.