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Displacive components of the low-temperature phase transitions in lawsonite

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ABSTRACT

The phase transitions in deuterated lawsonite were investigated with high-resolution, time-of-flight neutron diffraction between 2 and 500 K. From the analysis of spontaneous strain data, the thermodynamics of the phase transition at 273 K are not changed by the deuteration process. Shifts in atomic positions with temperature indicate continuous changes for a framework oxygen and for one of the deuterium atoms, whereas for the other deuterium atom, a more discontinuous behavior was observed in the average structure. Comparison of O···D and O···O bond lengths with IR data from a non-deuterated lawsonite permits a detailed analysis of assignments of O-H stretching modes.