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Spontaneous strain variations through the low temperature phase transitions of deuterated lawsonite

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ABSTRACT

High resolution neutron powder diffraction has been used to determine lattice parameter variations of deuterated lawsonite across the *Cmcm* ↔ *Pmcn* and *Pmcn* ↔ $P2_1cn$ phase transitions, in the temperature interval 1.6–505 K. The variations are reversible through heating and cooling cycles. Strain analysis, based on a displacive model of the transitions with saturation temperatures to describe the temperature-independent behavior as $T \rightarrow 0$ K, shows that the data are consistent with a tricritical transition at 271 ± 2 K and a second-order transition at 155 ± 1 K. Comparisons with strains from published dilatation data for a natural (hydrogenated) sample highlight aspects of the transitions that are most dependent on the behavior of protons in the structure. Replacing H by D causes the low temperature transition point to be increased by ~27 K and an anomaly in the strain evolution of the *Pmcn* transition to increase from ~225 to ~250 K. The transition point of the high-temperature transition remains the same within ± ~2 K. We conclude that proton ordering and displacive contributions are both important in the 271 K transition, though with the displacive component providing the initial symmetry-breaking mechanism. Structural changes that are more dependent on the behavior of H or D become important ~20–50 K below this. Strains for the *Pmcn* ↔ $P2_1cn$ transition are consistent with a transition driven by a single order parameter. The data are used to determine values for strain/order parameter coupling coefficients for calculation of elastic anomalies due to the phase transitions.