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Order parameter variation through the $C2/m$-$P2_1/m$ phase transition in cummingtonite

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ABSTRACT

The $C2/m$-$P2_1/m$ phase transition in natural cummingtonites, with different compositions, has been investigated by single-crystal X-ray diffraction and powder absorption IR spectroscopy. Variations in the intensity of type *b* (superlattice) reflections above room temperature are consistent with the transition being thermodynamically continuous and conform to the solution to a 2-4-6 Landau potential. Parameters extracted from IR spectra collected both above and below room temperature suggest that the local structural evolution differs slightly from the average macroscopic behavior observed by X-ray diffraction. Changes in wavenumber of an isolated absorption band at ~1130 cm^{-1} and changes in the integrated intensity of a band at ~760 cm^{-1} can be described by the solution to a 2-4 Landau potential with saturation below room temperature. Absorption bands due to O-H vibration and libration, however, appear to show discontinuities in the variation of their wavenumbers at the transition point. A local mechanism for the transition might involve a framework distortion providing the main driving force, with coupling to an order-disorder process for the protons.