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Order and miscibility in the otavite–magnesite solid solution

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Abstract

The effects of cation substitution and ordering in the otavite ($CdCO_3$)–magnesite ($MgCO_3$) solid solution have been investigated on samples synthesized at 1 GPa in the temperature range 500–800 °C for run durations up to 120 h. A complete, disordered solid solution, with $R\bar{3}c$ symmetry, was obtained at 800 °C, whereas Mg and Cd show partial ordering within the cadmium dolomite stability field, with $R\bar{3}$ symmetry, at intermediate compositions in the temperature range 500–650 °C. Rietveld refinements for X-ray diffraction data show that variation of the *a*-axis is linear as a function of composition, independent of the degree of order, whereas the *c*-axis shows a positive deviation from linearity as a function of composition, decreasing with increasing degree of order. Octahedral bond distances of the 800 °C series vary linearly with composition. Site occupancies were used to determine the long-range order parameter, *Q*, for samples with $R\bar{3}$ symmetry. Q^4 varies linearly as a function of temperature, suggesting a tricritical phase transition with a critical transition temperature T_c of 702(10) °C. EDX-TEM compositional microanalyses of samples within two-phase regions are in good agreement with Rietveld refinements, and allow better constraint of phase boundaries.

Keywords: X-ray powder diffraction, otavite–magnesite solid solution, carbonates, phase transition, cation ordering