Supporting Information

The Effect of Stoichiometry, Mg-Ca Distribution, and Iron, Manganese, and Zinc Impurities on the Dolomite Order Degree: A Theoretical Study

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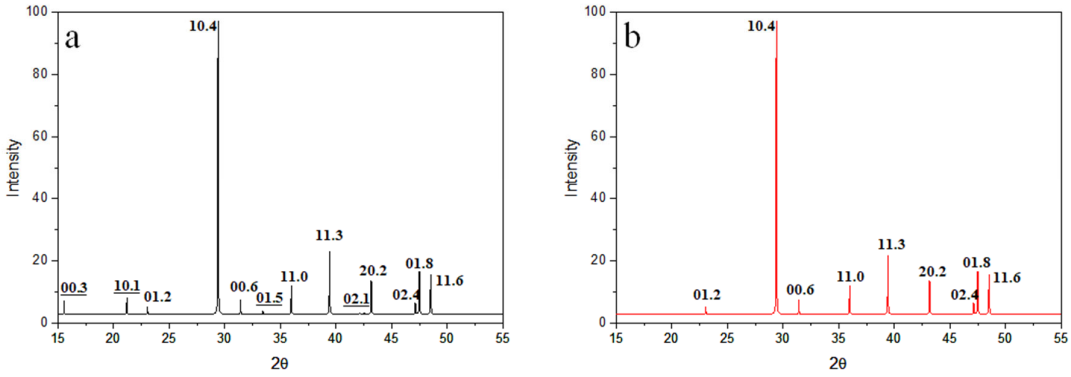

Figure S1. Diffractograms calculated with the RIETAN-FP code (Izumi and Momma, 2007, [19]) for a stoichiometric dolomite structure: (**a**) fully ordered: $x_{Mg} = 1$; (**b**) fully disordered: $x_{Mg} = 0.5$. In both diffractograms superstructure indexes appear underlined. Calculations have been conducted from a calcite structure (Maslen et al., 1995, [18]) as starting structure.

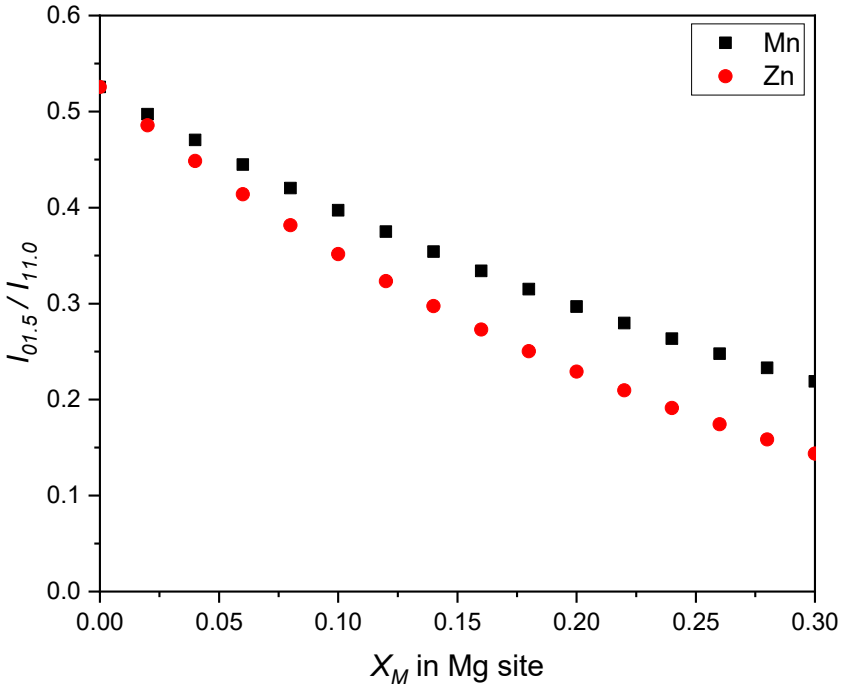

Figure S2. $I_{01.5}/I_{11.0}$ versus X_M (M = Mn or Zn) for dolomites with Mn and Zn impurities in the Mg site.