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The Mn, Mg-intracrystalline exchange reaction in donpeacorite ($Mn_{0.54}Ca_{0.03}Mg_{1.43}Si_2O_6$) and its relation to the fractionation behavior of Mn in Fe, Mg-orthopyroxene

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ABSTRACT

The equilibrium intracrystalline distribution of Mn and Mg between the M1 and M2 sites of a Mn-rich/Fe-free orthopyroxene (donpeacorite) was investigated by means of annealing experiments at temperatures between 980 and 800 °C and single-crystal X-ray diffraction. The data show that Mn, as does Fe^{2+} in Fe-Mg orthopyroxene, preferentially orders at the M2 site. However, comparison of the distribution coefficient $k_{D(Mn\text{-}Mg)}$ determined in this study with k_{D^*} measured for Fe-Mg orthopyroxene shows that Mn has a much stronger preference for the M2 site relative to Fe^{2+}. This result implies that the practice to partition Fe^{2+} + Mn = Fe* as one species, typically implemented to determine the quenched-site occupancies in Fe-rich/Mn-poor orthopyroxene, should be abandoned and that Mn should be considered totally ordered at M2. The partitioning method, i.e., Fe vs. Fe*, has implications for the determination of cooling rates from the observed ordering state of orthopyroxene, particularly for Fe-poor compositions (Fs < 0.16).