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Reverse Monte Carlo Modeling of Pair Distribution Function Data as a Tool for Separating the Coordination Environments of Multiple Atoms Disordered Over a Single Site

GRAHAM KING, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, REBECCA RICCIARDO, JENNIFER SOLIZ, PATRICK WOODWARD, Department of Chemistry, Ohio State University, FARSHID RAMEZANIPOUR, JOHN GREEDAN, Department of Chemistry, McMaster University —

The local structures of 8 perovskite compounds which contain equal concentrations of 2 transition metal cations disordered over the B-sites have been investigated using reverse Monte Carlo (RMC) modeling of neutron pair distribution function (PDF) data. Such compounds are known to display a number of interesting magnetic and electronic properties which, due to the cation disorder, cannot be correlated with the average long range structure and so remain poorly understood. In compounds with B=Mn/Ru there exists a valence degeneracy between Mn^{3+}/Ru^{5+} and Mn^{4+}/Ru^{4+}. We demonstrate that the RMC method can be used as an effective tool to separate out the individual coordination environments of these cations and also to monitor the relative concentrations of the different oxidation states. We find that the valency ratio is governed by the size of the A-site cations. In a different series of Sr_2FeMnO_{6-x} perovskites we find that locally the structures are quite different from the average cubic structures, with the local coordination environments more closely resembling those of the brownmillerite structure. In all compounds the octahedra containing Mn^{3+} are Jahn-Teller distorted, even if this distortion is not evident in the average structure.

Graham King
Los Alamos National Laboratory

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