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The description of Al, Si ordering in aluminosilicates using the cluster variation method

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Abstract

The cluster variation method (CVM) for determining the thermodynamics of both short-range and long-range order in this study was extended to complex aluminosilicate minerals. Using recently developed algorithms for the maximization of cluster entropies, it is possible to construct high-order cluster variation approximations for Ising lattices of complex topology. This study gives the essentials of developing CVM models for the Al, Si nets of nepheline, leucite, feldspar, and cordierite. The robustness of the method is demonstrated by its ability to reproduce quantitatively recently published results of Monte Carlo simulations of Al, Si ordering in the Ising model with feldspar topology. The future prospects for the application of CVM to aluminosilicates are discussed.