Molecular dynamics simulation of albite

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Molecular dynamics (MD) simulations for the phase transitions of albite were carried out using the structures with various Al/Si ordering parameter. The data were analyzed using two kinds of order parameters, which represent the lattice distortion and Al/Si ordering. The results show that the symmetry reduction from C2/m to C-1 was dominated by 2nd order transition due to both the lattice distortion and the Al/Si ordering, and that there was no thermal crossover between high- and low-albite.