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The ab initio study of the stability of low temperature Al/Si ordered albite, $NaAlSi_3O_8$

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ABSTRACT

The energetics of different ordering schemes for $NaAlSi_3O_8$ (albite) were investigated by both empirical potential and ab initio methods. These computations indicate that the ordered structure of natural low albite, in which aluminum atoms reside on the T_{10} site, is favored by 30 meV (2.9 kJ/mol) over the corresponding structure in which aluminum atoms are ordered onto the T_{20} site. Permissible lattice relaxation of the T_{10} structure, with an associated substantial decrease in the γ lattice angle, is unique to the T_{10} structure and appears to be responsible for its substantially lower enthalpy.