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Rigid unit modes in crystal structures with octahedrally coordinated atoms

KENTON D. HAMMONDS,[1,2] ANNE BOSENICK,[2,3] MARTIN T. DOVE,[2,*] AND VOLKER HEINE[1]

[1]Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 OHE, U.K.
[2]Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.
[3]Mineralogisch-Petrographisches Institut, Christian-Albrechts Universität, Olshausenstrasse 40, D-24098, Kiel, Germany

ABSTRACT

The rigid unit mode analysis was initially developed to understand the phase transitions in aluminosilicate minerals containing corner-linked tetrahedra. Here the model is applied to a range of minerals with crystal structures that can be described as frameworks of linked octahedral and tetrahedral units, including garnet, sillimanite, titanite, and ellenbergerite. Consistent with a constraint analysis, there are no rigid unit modes in these minerals. Generalizing these results suggests that there will not be any easy ways to distort structures that have frameworks containing octahedral units. This result explains why polyhedral-tilting displacive phase transitions are not common in such minerals, whereas they occur in most aluminosilicate minerals containing only tetrahedral units. It also explains that it will be necessary for the tetrahedra and octahedra to distort when solid solutions are formed.