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Lattice-dynamical evaluation of thermodynamic properties and atomic displacement parameters for beryl using a transferable empirical force field

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Abstract

Using empirical potentials derived from fitting the vibrational frequencies of a group of silicates and oxides, and crystallographic information, a Born-von Karman rigid-ion lattice-dynamical model has been applied to the whole Brillouin zone in beryl. The Raman and infrared spectra are satisfactorily reproduced and interpreted by these calculations; there is also very good agreement with atomic displacement parameters derived from accurate crystal-structure refinement by various authors and with experimental values of thermodynamic functions for the anhydrous phase at different temperatures. The agreement of our calculations with experimental data of independent origin and nature demonstrates the potential of such a procedure.