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Vibrational spectroscopy of brucite: A molecular simulation investigation

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ABSTRACT

We have modeled the vibrational spectrum of brucite, the common phase of magnesium hydroxide, at 1 bar (10^5 Pa) by two separate techniques: molecular dynamics simulation and vibrational mode analysis. Molecular dynamics simulation of a model supercell provides information (from the power spectrum of the atomic velocity autocorrelation function) about the frequencies and directions of atomic thermal motions, using a defined energy force field. Vibrational mode analysis gives complementary information about the frequencies, nature, and infrared and Raman activity of the computed modes of the same system. Using both methods we find (in addition to the spectroscopically active modes) inactive modes up to around 1000 cm^{-1}, corresponding to MOH bending (OH rotational) motions. We invoke these modes to explain the published inelastic neutron scattering data, and suggest that their relatively high frequency is an inevitable consequence of repulsive interactions between neighboring H atoms.

Keywords: Brucite, magnesium hydroxide, infrared, molecular dynamics, neutron scattering, vibrational spectra