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Combined inelastic neutron scattering and solid-state density functional theory study of dynamics of hydrogen atoms in muscovite $2M_1$

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Abstract

Inelastic neutron scattering (INS) was used to study dynamics of the hydrogen atoms in natural $2M_1$ muscovite in the 150–1200 cm^{-1} energy range. The resultant INS spectra are interpreted by means of solid-state density functional theory calculations covering both normal mode analysis and molecular dynamics. While signatures of the Al-O-H bending modes were found over the whole energy transfer range, the dominant contributions were observed between 800–1000 cm^{-1}. The modes assigned to the in-plane movements of the respective hydrogen atoms are well defined and always appear at high energies. In contrast, the modes corresponding to the out-of-plane movements are spread over large energy transfer ranges, extending down to the region of external (lattice) modes. The positions of the high-energy modes contributing to the INS band at ~907 cm^{-1} depend on the distance of respective hydrogen atoms to the nearest oxygen atom of the basal net and its polarity.

Keywords: Inelastic neutron scattering, muscovite, DFT, vibrational spectra, molecular dynamics