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The vibrational spectrum of lizardite-1*T* [$Mg_3Si_2O_5(OH)_4$] at the Γ point: A contribution from an ab initio periodic B3LYP calculation

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Abstract

The vibrational spectrum of lizardite at the Γ point has been calculated with ab initio methods, using a hybrid HF/DFT Hamiltonian (B3LYP). Apart from a few bending modes involving hydrogen motion, very good agreement has been found between calculated and experimental infrared and Raman spectra of the mineral. The anharmonic correction to the OH-stretching modes proved to be crucial for a correct evaluation of their frequencies and, on average, it amounts to a lowering of about 150 cm^{-1} with respect to the values computed within the harmonic approximation. LO-TO splitting effects had to be taken into account for a correct interpretation of the data obtained from infrared spectra on powder samples. The calculation can be used either to confidently identify which bands in the experimental spectra do correspond to fundamental vibrational transitions or to unequivocally assign them to specific normal modes.

Keywords: Lizardite, vibrational frequencies, normal modes, computational modeling