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Vibrational and magnetic properties of crystalline CuTe2O5

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Abstract

© 2014, Pleiades Publishing, Inc. In the present work we have performed an ab initio calculation of vibrational properties of CuTe2O5 by means of density functional theory (DFT) method. One has compared calculated values with known experimental data on Raman and infrared spectroscopy in order to verify the obtained results. Lattice contribution to the heat capacity obtained from the ab initio simulations was added to magnetic contribution calculated from the simple spin Hamiltonian model in order to obtain total heat capacity. Obtained results are in good agreement with the experimental data. Thus, the DFT methods could complement the experimental and theoretical studying of low-dimensional magnetic systems such as CuTe2O5.

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