The Study of Lattice Dynamics in Dimerized Quantum Magnets with Chain-Like Crystal Structure

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Abstract. This work is devoted to the comparative study of the lattice specific heat of Cu(*en*)$(H_2O)_2SO_4$, Cu(*en*)$_2SO_4$ and Cu(*en*)$_2CrO_4$, where *en* = ethylenediamine - $C_2H_8N_2$. Previous studies on the effects of spatial anisotropy of exchange coupling within the magnetic layer showed that quasi-one-dimensional polymer structures based on Cu(II) ions, Cu(*en*)$(H_2O)_2SO_4$ and Cu(*en*)$_2SO_4$ represent realizations of spin 1/2 Heisenberg model on the spatially anisotropic zig-zag square lattice and the dimerized square lattice, respectively. The substitution of S-Cr in isomorphic Cu(*en*)$_2SO_4$ and Cu(*en*)$_2CrO_4$ introduces differences in lattice specific heat. The description of the heat capacity of the lattice up to room temperature was carried out considering the contribution of acoustic phonons within the Debye model and optical phonons using Einstein approximation. Deviations of the Debye model from the lattice heat capacity are already observed above 15 K for all compounds, for Debye temperatures θ_D = 146 K, 101 K and 94 K for Cu(*en*)$(H_2O)_2SO_4$, Cu(*en*)$_2SO_4$ and Cu(*en*)$_2CrO_4$, respectively. The effect of acoustic and optical modes on magnetic correlations in these systems is also discussed.