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Modelling the magnetic exchange interactions relative to inelastic neutron scattering results in the quantum antiferromagnet atacamite

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An experimental inelastic neutron scattering (INS) study on atacamite (Cu2Cl(OH)3) has been performed using Pelican to verify previous density-functional theory (DFT) calculations of its magnetic exchange interactions. INS reveals two dispersive spin wave modes along the H direction. Comparison with linear spin wave theory (LSWT) modelling indicates a frustrated zigzag-chain system along the crystallographic a direction. Additionally, the INS data reveals a spin wave gap along the H direction of at least 0.75 meV. LSWT modelling reveals that an additional perturbative term in the Hamiltonian is essential to reproducing the experimental spin wave gap. At first glance, the zigzag chain is not congruent with previous DFT results. We propose that the zigzag chain represents an effective model which is valid at low temperature, whereas the previously proposed sawtooth chain represents a Hamiltonian for atacamite whose characteristics are only present in a high-temperature regime.

Topics

Magnetism and Condensed Matter

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