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Spin Dynamics of $\text{Ba}_5\text{Ru}_3\text{O}_{12}$: An Inelastic Neutron Scattering and Machine Learned Force-Field Study

We have Performed an inelastic neutron scattering (INS) investigation on the trimer ruthenate $\text{Ba}_5\text{Ru}_3\text{O}_{12}$, that undergoes long-range antiferromagnetic ordering at $T_N = 60$ K. The INS spectra suggest two distinct spin-wave excitations one at 5.6 meV, which is less intense and a broader intense excitation around 10-15 meV. Notably, these magnetic excitations persist well above T_N , indicating short-range correlations in the trimer network. We have modelled this spectra using linear spin-wave theory (SpinW) in combination with machine-learning force-field (MLFF) calculations which suggest that $\text{Ba}_5\text{Ru}_3\text{O}_{12}$ hosts strong magnetic frustration arising from competing nearest and next-nearest-neighbor exchange interactions, exchange anisotropy, and strong spin-orbit coupling. These competing interactions stabilize a non-collinear magnetic structure which makes this compound different from all other compounds that belongs to the same ruthenate trimer family. Furthermore, our theoretical calculations of the isolated Ru_3O_{12} trimer ground state are consistent with the experimentally observed excitation energies, providing a unified understanding of the magnetic dynamics in $\text{Ba}_5\text{Ru}_3\text{O}_{12}$.

Session

Magnetism

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