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Insights Nuanced Magnetic Structure, Spin Superexchange, and Single-Ion Anisotropy in Perovskite-like $CaCu_3Ti_4O_{12}$ via Neutron Scattering Techniques

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This comprehensive study delves into the complex magnetic properties and interactions of the perovskite-like compound $CaCu_3Ti_4O_{12}$, employing advanced neutron scattering techniques and resonant inelastic X-ray scattering (RIXS) to explore the underlying spin-orbital coupling and single-ion anisotropy. By synthesizing high-quality single crystals and utilizing a four-circle neutron diffractometer, we capture sufficient magnetic reflections to accurately determine the magnetic structure. In-depth investigations using a neutron three-axis spectrometer reveal the exchange interactions and anisotropic energies, elucidating the spin wave spectrum and highlighting the significant role of indirect exchange interactions mediated through Ti^{4+}. Additionally, the RIXS measurement uncovers the \textit{dd}-excitations, helping to establish the relationship along individual axes and confirming the anisotropic energies observed in the spin wave analysis. This research offers clear insights into both the collective spin-orbital coupling as modeled by the Kugel-Khomskii framework and the specific contributions of self-spin-orbit coupling concerned with single-ion anisotropy within $CaCu_3Ti_4O_{12}$. These findings contribute to a deeper understanding of magnetic interactions in systems with strong spin-orbital correlations and pave the way for future research into the delocalization of orbital excitation.

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