

Inelastic Neutron Scattering of Lanthanoid-Radical Molecular Nanomagnets

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Single-molecule magnets (SMMs) are materials which exhibit slow relaxation of magnetization and quantum tunneling of molecular origin. These properties make them promising for future applications in high-density data storage, as qubits in quantum computing, and in molecular spintronics.^[1] The best performing SMMs are complexes of the late trivalent lanthanoid (Ln(III)) ions. The energy barrier to reversal of magnetization here stems from the crystal field (CF) splitting of the spin-orbit coupled ground state with total angular momentum J . The identity and geometry of the coordinated ligands determines the relative order, energy and composition of these CF states, such that appropriate choice of ligands can tune the CF splitting and therefore the SMM behaviour.

Incorporation of organic radicals can be used to improve SMM behaviour, by shifting quantum tunneling of the magnetisation, a through-barrier relaxation pathway, from zero field.^[2] The nature of magnetic exchange coupling between a Ln(III) ion and another paramagnetic moiety is, however, hard to determine, and often cannot be determined directly due to the large spin-orbit coupling inherent in many Ln compounds. Inelastic neutron scattering is a powerful experimental technique for directly measuring the CF splitting and exchange coupling in Ln(III) compounds.^[3]

Our group has been studying a family of compounds with formula $[\text{Ln}(\text{dbsq})\text{Tp}_{<\text{sub}>2</\text{sub}>}]$, $\text{Tp}_{<\text{sup}>-</\text{sup}>} = \text{tris}(\text{pyrazolyl})\text{borate}$, $\text{dbsq}_{<\text{sup}>-</\text{sup}>} = 3,5\text{-di-tert-butyl-semiquinonate}$, which show exchange coupling between the Ln(III) ion and the dbsq organic radical.^[4] We have studied the INS spectra the Ln = Tb, Ho, Er, and Yb analogues on the cold neutron time-of-flight spectrometer PELICAN, as well as their magnetic properties. We observe temperature dependent CF transitions, which are compared to the energy level splitting obtained from electronic structure calculations, as well as exchange transitions in two analogues, which give us both the magnitude of and spatial information about the exchange coupling in this family of compounds.

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Level of Expertise

Student

Speakers Gender

Female

Do you wish to take part in the poster slam

No

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