Experimental report

11/07/2023

Proposal: 4-06-16 **Council:** 4/2020

Title: Low-lying magnetic excitation of cyclic molecular magnet {Cr8Y8}

Research area: Physics

This proposal is a new proposal

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Samples: [Cr8Y8(mda)16(CH3COO)8(NO3)8]
Fe8Y8N21O96C122H303

Instrument	Requested days	Allocated days	From	To
IN16B	3	2	25/08/2021	26/08/2021

Abstract:

A hexadenuclear heterometallic wheel-like molecular cluster {Cr8Y8} was synthesized. The magnetic susceptibility shows that the magnetic interaction is ferromagnetic between CrIII ions. {Cr8Y8} provides a rare example of ferromagnetic rings. Specific heat data show distinct Schottky anomalies, indicating the presence of low-lying magnetic excitations. The energy gaps resolved from specific heat data and INS data are partially consistent with each other, and can be approximated by a single-J model. Specific heat data also shows a small energy gap about 9.3 micro eV, which may be due to the zero-field splitting of the S=12 ground state. This energy gap could not be measured in our previous INS measurements due to the limitation of instrumental resolution. We propose to use high resolution backscattering spectrometer IN16B to determine precisely this low-lying zero-field splitting in {Cr8Y8}.

Experimental report: Low-lying magnetic excitation of cyclic molecular magnet {Cr_8Y_8} (Proposal 4-06-16)

We have synthesized hexadenuclear heterometallic molecular wheel {Cr_8Y_8} powders. Magnetic study shows that the nearest-neighbor Cr^{3+} moments are ferromagnetically coupled. The specific heat measured at various fields can be well fitted with a lattice term ($\sim T^3$) and a multi-level Schottky term. At zero external field, the data fit yields a small energy gap of ΔE_{ZFS} = 9.3 μeV, which may originate from the zero-field splitting (ZFS) of the $|S = 12\rangle$ ground state. However, our previous INS measurements could not measure an energy gap as small as 9.3 μeV. The aim of this experiment is to unambiguously measure the energy of the possible ZFS of $|S = 12\rangle$ ground state of {Cr_8Y_8} by means of high-resolution backscattering spectrometer IN16B.

We have measured inelastic neutron scattering spectra from {Cr_8Y_8} powders on D16B at various temperatures from 2 to 20 K. The INS spectra for 2 and 20 K are shown in the figure below. The spectra can be well fitted by a Gaussian function to describe the strong central elastic line due to instrumental resolution and incoherent scattering, a quasielastic term (purple dash line), and an INS term (green dash line) to describe the inelastic peaks at ~5 μeV. The INS peaks at ~5 μeV are probably due to the zero-field splitting. However, the rotational tunneling of methyl groups may also lead to such INS signals. Further analysis is underway.