High Magnetic Field Heat Capacity on Fe-Based Molecular Magnets

Heat capacity measurements of the molecular magnets {Fe_{16}} and {Fe_{12}} were performed in magnetic fields up to 14.5 T. Isothermal heat capacity data, collected at 1.8 K as a function of the magnetic field, reveal broad anomalies consistent with the presence of weak crystal-field anisotropy and magnetic interactions.

Superexchange interactions in the molecular clusters {Fe16} and {Fe12} lead to the stabilization of ground states with spin values $s = 20$ and $s = 8$, respectively, as shown in previously measured magnetization data. In addition, {Fe16} exhibits clear evidence of a dipolar-coupling-driven phase transition below 1 K, as revealed by heat capacity measurements at low magnetic fields. This behavior is analogous to that observed in the related compound {Fe17} [1], [2].

During the experiments conducted at HFLSM in the period from January 4 to March 1, 2026, new isothermal heat capacity data were collected at 1.8 K for both Fe-based molecular magnets. Magnetic fields of up to 14.5 T, generated by the 15 T superconducting magnet (15TSM), were used in combination with the heat capacity setup developed by Dr. M. Akaki.

Fig. 1 shows the new data for {Fe16}, revealing a broad feature centered around $B = 3$ T, in agreement with measurements previously obtained using a PPMS system (Quantum Design) for magnetic fields up to 7 T. In the new data recorded for $B > 7$ T, no additional anomalies are observed.

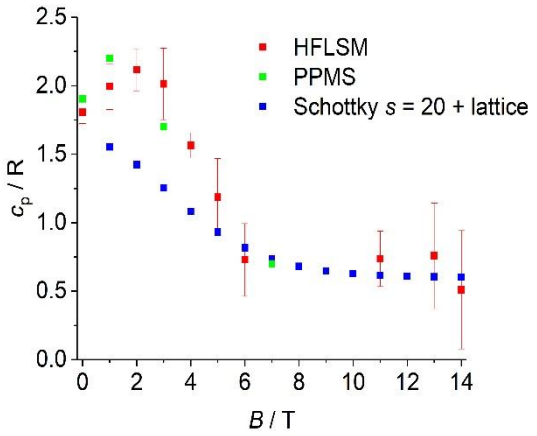

Fig. 1 Isothermal heat capacity data for {Fe_{16}}.

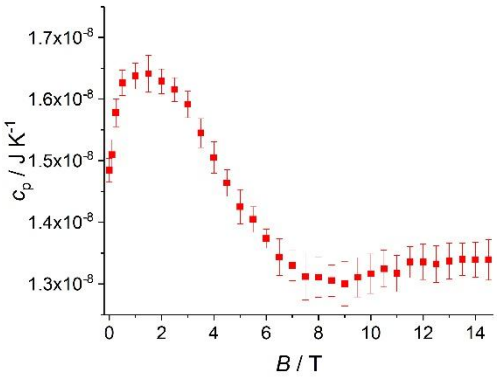

Fig. 2 Isothermal heat capacity data for {Fe_{12}}.

Similarly, Fig. 2 presents the new data for {Fe12}. A broad anomaly is observed around $B = 2$ T, while for fields above 8 T the heat capacity remains essentially constant, with no evidence of additional magnetic features within the studied field range. This behavior can be satisfactorily reproduced by parameterizing the interactions among the twelve Fe ions using six different exchange constants obtained from DFT analysis (not shown here). These results will be reported in a forthcoming publication that is currently in preparation.

References

[1] Evangelisti, M.; et al. Tunable dipolar magnetism in high-spin molecular clusters. Physical Review Letters, vol. 97, no. 16, pp. 167202, 2006.

[2] Gass, I.A.; et al. Cryogenic magnetocaloric effect in the Fe17 molecular nanomagnet. Polyhedron, vol. 52, pp. 1177–1180, 2013.

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