High-Frequency/Field Electron Paramagnetic Resonance and High-Field Magnetization Studies on Wheel-like Clusters

Abstract: A family of 3d-4f wheel-like clusters {Fe_8Ln_8} (Ln = Gd, Tb, Dy, Ho, Er) and a giant 4f wheel-like cluster {Dy_{20}} were isolated and studied by high-frequency/field electron paramagnetic resonance (HF-EPR) and high-field magnetization. HF-EPR spectra aere observed in {Fe_8Ln_8}, which can help to exact the magnetic exchange-coupling constants, while magnetic hysteresis loops were observed for {Dy_{20}}, indicating a wheel-like single-molecule magnet.

HF-EPR spectra of polycrystalline [Fe_8Ln_8] (Ln =Gd, Tb, Dy, Ho, Er) were collected in a wide frequency range between 135 and 405 GHz at 4.2 K. Wheel-like clusters display fantastic magnetic properties because of their non-collinear arrangement of their spins.

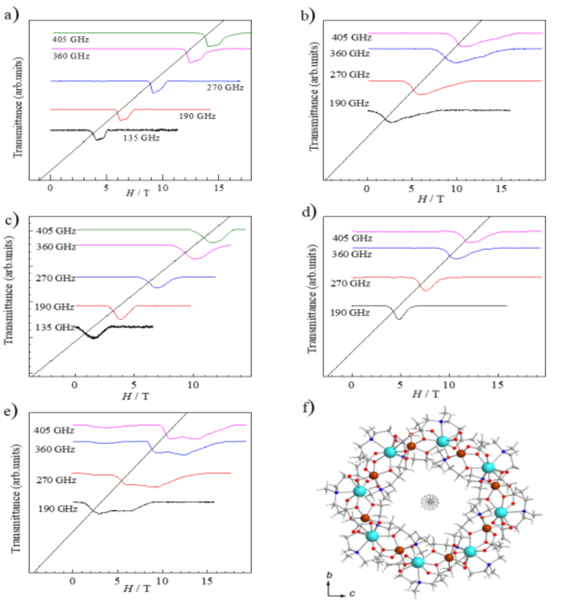

Fig. 1 Selected HF-EPR spectra of [Fe_8Ln_8] measured at 4.2 K [Ln = (a) Gd, (b) Tb, (c) Dy, (d) Ho and (e) Er]. The spectra are offset in a linear scale of the frequency. Straight line are drawn from the linear fitting in the frequency field plot. (f) Ball-and-stick modes of the molecular structures of {Fe_8Ln_8} wheels.

Table 1 The level-crossing fields (H_C) and energy gap (ΔE) from linear fitting in the frequency field plot for {Fe_8Ln_8} wheels.

	Fe_8Gd_8	Fe_8Tb_8	Fe_8Dy_8	Fe_8Ho_8	Fe_8Er_8
H_c / T	-0.60	-4.35	-3.30	-2.18	-4.02
ΔE/GHz	16.45	111.72	88.32	58.45	105.35

Fig.1 shows HF-EPR spectra at 4.2 K for {Fe_8Gd_8} (1a), {Fe_8Tb_8} (1b), {Fe_8Dy_8} (1c), {Fe_8Ho_8} (1d), and {Fe_8Er_8} (1e) with crystal structure for {Fe_8Ln_8} (1f). With HF-EPR studies, the level-crossing field (H_C), together with the g factor and energy gap (ΔE) can be determined from extrapolation in these plots (Figure 1 and table 1). Combined with the magnetic susceptibilities, we are going to determine the exchange couplings between Fe(III) ions and Ln(III) ions with the method reported by Prof. Hiroyuki Nojiri et al .[1-2].

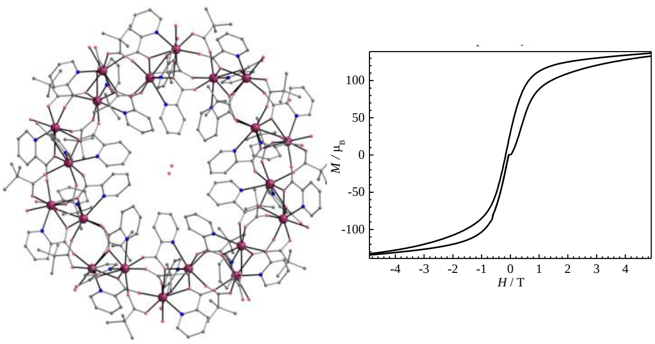

Fig. 2 (a) Molecular structure of {Dy_{20}}. Color code: Ln, purple; O, pink; N, blue; C, grey. (b) Magnetic hysteresis loop at 0.45 K for {Dy_{20}}

The structure of wheel-like cluster {Dy_{20}} was shown in the Fig 2a. At 0.45 K, magnetic hysteresis loops can be clearly observed (Fig 2b), which is indicative of a single-molecule magnet. With magnetic susceptibilities and theoretical studies, we will have a clear understanding about electronic structure in those wheel-like clusters. With better and clearer understanding of the magneto-structural correlation, electronic structure and energy levels of those wheel-like clusters, single-molecule toroidal behavior may be clarified. We wish to publish three research papers in high-profile journals using these results.

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References

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