## High-Temperature Lanthanide Single-Molecule Magnets

Richard A. Layfield

Department of Chemistry, School of Life Sciences, University of Sussex, Brighton, BN1 9QJ, U.K.

## R.Layfield@sussex.ac.uk

Single-molecule magnets (SMMs) are metal-organic compounds that display magnetic hysteresis below a blocking temperature,  $T_{\rm B}$ .<sup>1</sup> Such materials have been proposed for numerous device applications, including as qubits in quantum computers.<sup>2</sup> We have interests in metallocene SMMs based on dysprosium, and, over the years, we have reported a few examples of such materials.<sup>3</sup>

Our work has shown that  $[Cp]^-$  ligands provide a strong axial crystal field that enhances the magnetic anisotropy of Dy<sup>3+</sup>, leading us to propose that a cation of the type  $[Cp_2Dy]^+$  should be an interesting synthetic target.<sup>4</sup> Recently, we described the properties of  $[(\eta^5-Cp^*)Dy(\eta^5-C_5/Pr_5)][B(C_6F_5)_4]$  ([1] $[B(C_6F_5)_4]$ ), which has  $T_B = 80$  K, making it the first (and, so far, only) SMM to display hysteresis above the boiling point of liquid nitrogen (Figure 1).<sup>5</sup>



**Fig. 1** Molecular structure of **1**, and frequency-dependence of the out-of-phase susceptibility, magnetic hysteresis at 2-75 K (sweep rate of 200 Oe  $s^{-1}$ ) and at 80 K (sweep rate of 25 Oe  $s^{-1}$ ) for [**1**][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>].

Having established the design principles required to optimize the SMM properties of dysprosium sandwich complexes, we now turn our attention to alternative ligand environments. Recent finding on SMMs containing cyclobutadienyl ligands, [Cb]<sup>2–</sup> will be described,<sup>6</sup> as will a 'bio-inspired' synthetic route to SMMs that resembles the chemistry of flavo-diiron nitric oxide reductase (FNOR).<sup>7</sup>

## Acknowledgements

RAL thanks the ERC for a Consolidator Grant, the University of Sussex, the EPSRC, the EU Marie Sklowdowska-Curie Actions and COST Actions, the Royal Society and the Newton Trust.

## References

- R. A. Layfield *et al. Chem. Rev.* 2013, *113*, 5110. (b) R. A. Layfield, *Organometallics*, 2014, 33, 1084. (c) J. M. Frost, K. L. M. Harriman, M. Murugesu, *Chem. Sci.* 2016, 7, 2470. (d) J.-L. Liu, Y.-C. Chen, M.-L. Tong, *Chem. Soc. Rev.* 2018, *7*, 2431.
- 2. A. Gaita-Ariño, F. Luis, S. Hill, E. Coronado, Nat. Chem. 2019, 11, 301.
- 3. B. M. Day, F.-S. Guo, R. A. Layfield, Acc. Chem. Res. 2018, 51, 1880.
- 4. (a) R. A. Layfield *et al. Angew. Chem. Int. Ed.* **2016**, *55*, 11082; (b) S. Gao *et al. Chem. Eur.–J.* **2016**, *22*, 12724.
- 5. R. A. Layfield *et al.* Science **2018**, 362, 1400.
- 6. R. A. Layfield et al. Chem.- Eur. J. 2018, 24, 16779, and unpublished results.
- 7. A. K. Bar, J. Tang, R. A. Layfield, manuscript in preparation.