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COMMUNICATION – Supporting Information

Ferromagnetic coupling in a chloride-bridged erbium single-molecule magnet

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Contents

1. General considerations:

All manipulations were carried out under an atmosphere of dinitrogen using standard Schlenk line and glovebox techniques. THF and diethyl ether were dried on an activated alumina column and stored on 3 Å molecular sieves for two days before use. $ErCl_3$ powder and COT were purchased from Aldrich and used as received. Elemental analyses were conducted by Midwest Microlab, Indianapolis, IN.

1.1 bis((u$_2$-chloro)-η^8-cyclooctatetraenyl)-bis(tetrahydrofuran)-erbium) (**1**) synthesis:

Dipotassium cyclooctatetraenide was prepared via the method published by Meihaus[1]. K_2COT (0.1259 g, 0.6904 mmol) in 10 mL THF was added, dropwise, to a stirring suspension of $ErCl_3$ (0.1889 g, 0.6904 mmol) in 5 mL THF over the course of 10 minutes. The addition must be performed slowly so as not to irreversibly produce $K[Er(COT)_2]$. After stirring for 12 hours the mixture was centrifuged (3200 rpm, 20 minutes) and the supernatant separated and dried *in vacuo*. The dried solids were suspended in 10 mL THF before heating to 100 °C in a sealed scintillation vial to form a clear pink solution. Diethyl ether was diffused into this solution to yield pink plates of **1** (0.1259 g, 48.2%). CHN analysis (found, calc.) for $C_{24}H_{30}Cl_2Er_2O_2$: C (37.51, 38.13); H (4.42, 4.00); N (0.00, 0.00).

2. Crystallographic information:

Single crystal X-ray data for **1** were collected at 100 K on a Bruker κ Diffractometer with a Mo Kα radiation source and an Apex II Area Detector. The structure was solved using direct methods *via* the SHELXT[2] routine and refined using full-matrix least-squares procedures with the SHELXL routine. Olex[2] was used as a graphical front-end[3].

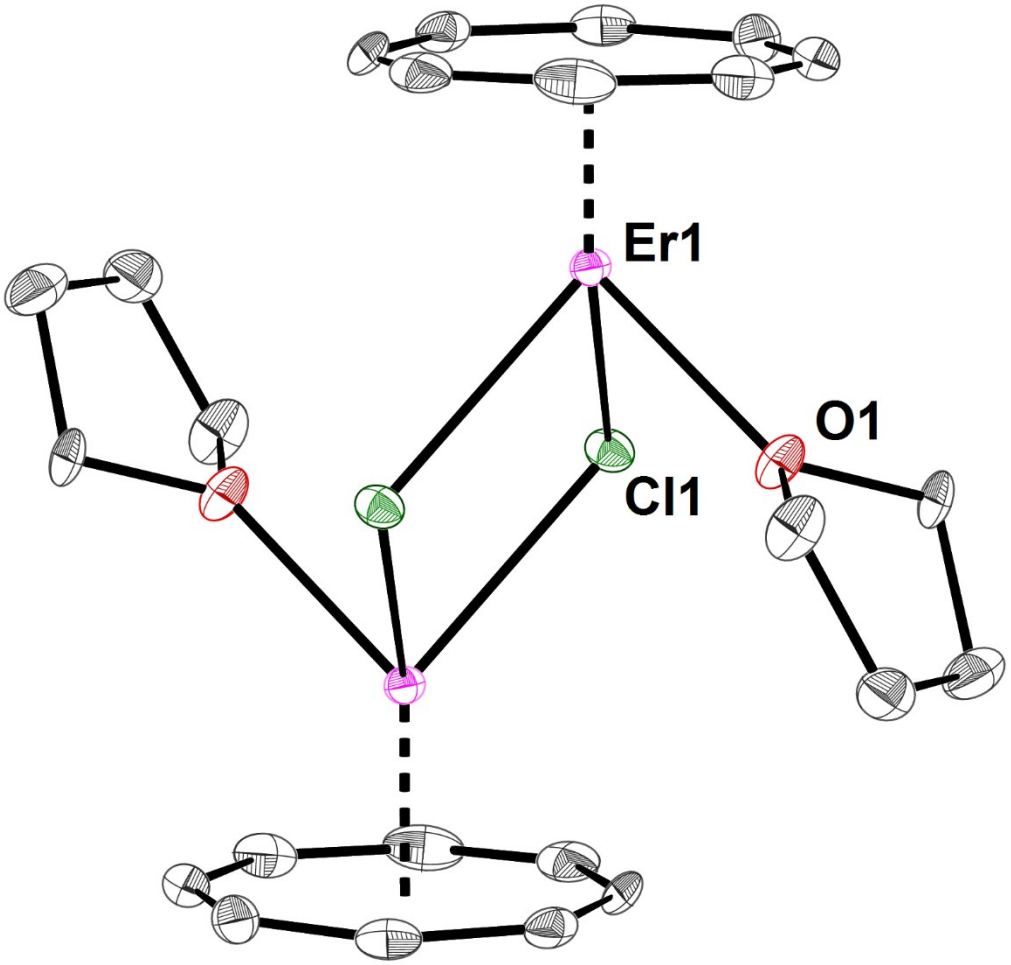

Figure S1. Solid-state ORTEP for **1**. The thermal ellipsoids are represented at 50% probability level. Hydrogen atoms have been omitted for clarity. Selected distances:
Er1-Cl1, 2.7014(2) Å; Er1-Cl1', 2.7046(2) Å; Er1-COT (centroid), 1.7538(1) Å; Er1-O1, 2.3367(1) Å; Er1-Er1', 4.0809(2) Å.

3. Magnetic analyses:

Magnetic analyses were conducted with a Quantum Design MPMS3 SQUID Magnetometer in DC scan mode. 21.8 mg of crystalline sample was sealed under vacuum in a custom quartz tube (D & G Glassblowing Inc.) with 4 mm inner-diameter. 29.0 mg of melted eicosane was added to the sample to abate torqueing and improve thermal conductivity during measurements. All acquired data were corrected for the diamagnetism of eicosane and the sample itself using Pascal's constants[4]. Temperature-dependence studies were performed at various ramp-rates to ensure phonon-bath mediated processes were not effecting the susceptibility.

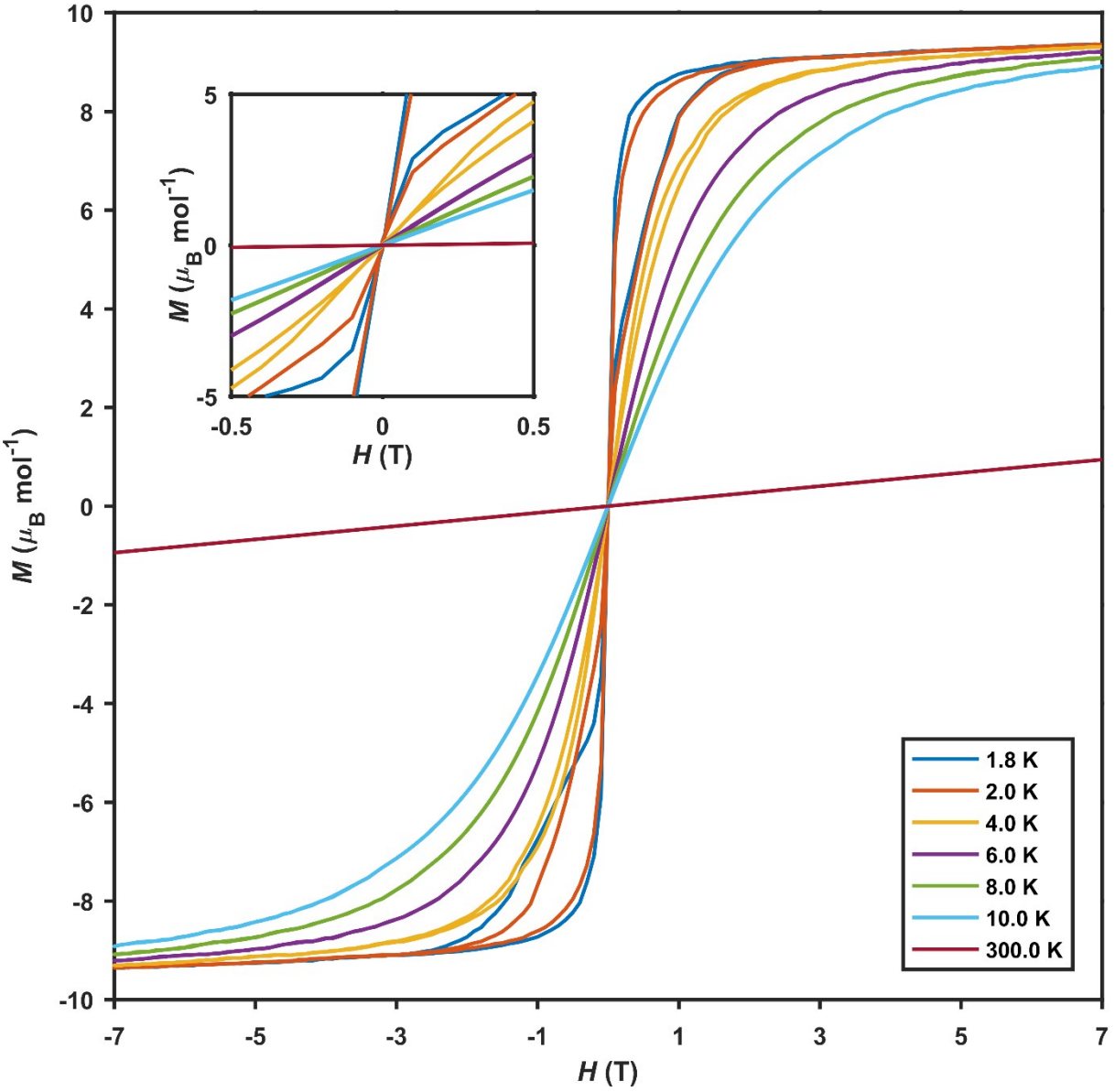

Figure S2. Isothermal magnetization of **1** measured between 1.8 and 300.0 K.

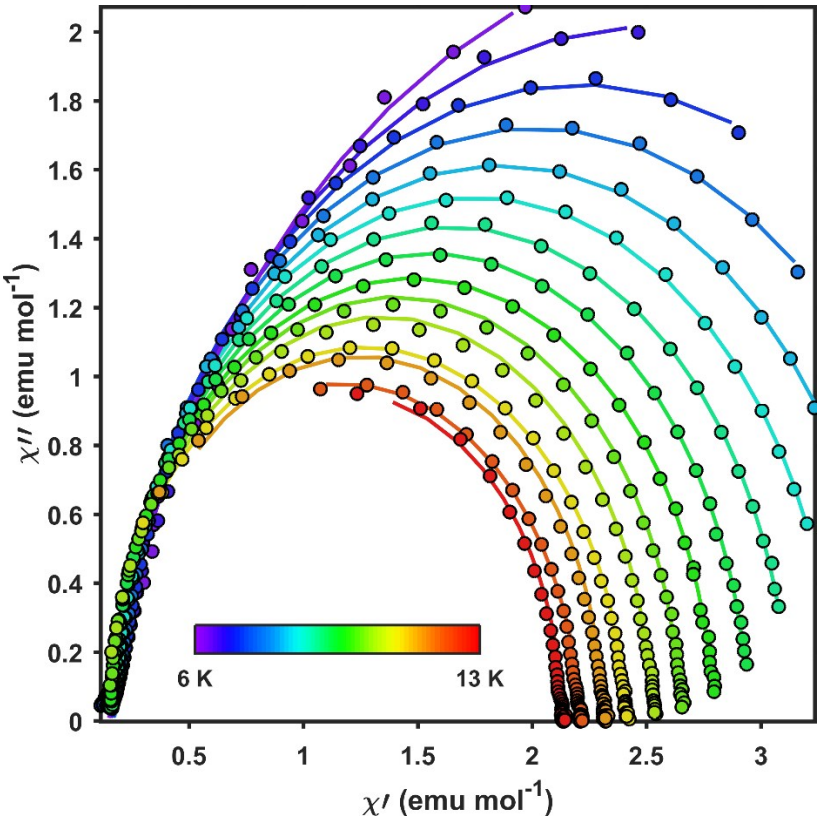

Figure S3. Cole-Cole plot of the zero-field ac susceptibility of **1** between 6 and 13K. Circles represent experimental data and solid lines are their corresponding fits.

4. References:

(1) Meihaus, K. R.; Long, J. R. Magnetic blocking at 10 K and a dipolar-mediated avalanche in salts of the bis(η8-cyclooctatetraenide) complex [Er(COT)2]-. *J. Am. Chem. Soc.* **2013**, *135* (47), 17952–17957 DOI: 10.1021/ja4094814.

(2) Sheldrick, G. M.; IUCr; S., W. K.; J., D. E.; S., D. M.; P., P. J.; G., G. M.; E., M. P. R.; A., D. L. R. M.; M., S. G. A short history of *SHELX*. *Acta Crystallogr. Sect. A Found. Crystallogr.* **2008**, *64* (1), 112–122 DOI: 10.1107/S0108767307043930.

(3) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.; K., S.; L., W.; G., P.; R., S. *OLEX2* : a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **2009**, *42* (2), 339–341 DOI: 10.1107/S0021889808042726.

(4) Bain, G. A.; Berry, J. F. Diamagnetic Corrections and Pascal's Constants. *J. Chem. Educ.* **2008**, *85* (4), 532 DOI: 10.1021/ed085p532.