

Supporting Information for:

A Promising New Route towards Single-Molecule Magnets Based on the Oxalate Ligand

Gong-Feng Xu,^{a,b} Qing-Lun Wang,^b Patrick Gamez,^c Yue Ma,^b Rodolphe Clérac,^{*d,e}
Jinkui Tang,^{*a} Shi-Ping Yan,^b Peng Cheng^b and Dai-Zheng Liao^{*b}

^a State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China. Fax: (+)86-0431-85262878; E-mail: tang@ciac.jl.cn

^b Department of Chemistry, Nankai University, Tianjin 300071, P. R. China. Fax: (+)86-022-23509957; E-mail: liaodz@nankai.edu.cn

^c Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, P. O. Box 9502, 2300 RA Leiden, The Netherlands

^d CNRS, UPR 8641, Centre de Recherche Paul Pascal (CRPP), Equipe "Matériaux Moléculaires Magnétiques", 115 avenue du Dr. Albert Schweitzer, Pessac, F-33600, France

^e Université de Bordeaux, UPR 8641, Pessac, F-33600, France

Experimental Section

An aqueous solution (20 mL) of K₂ox·H₂O (0.184 g, 1 mmol) and K(HBpz₃) (1.01 g, 4 mmol) was added to a stirred aqueous solution (20 mL) of DyCl₃·6H₂O (0.754 g, 2 mmol). The solution was stirred for 5 min, and then cooled in a refrigerator overnight. The resulting white precipitate was filtered off, washed three times with water, and dried under vacuum. The crude product was recrystallized from dichloromethane-acetonitrile several times (yield = 43%). Single crystals, suitable for X-ray diffraction analysis, were obtained by slow evaporation of the solvent from a solution of the compound in dichloromethane-acetonitrile. Anal. Calcd for C₄₃H₄₈N₂₆O₄B₄Cl₂Dy₂: C, 36.06; H, 3.38; N, 25.43. Found: C, 35.37; H, 3.24; N, 25.86.

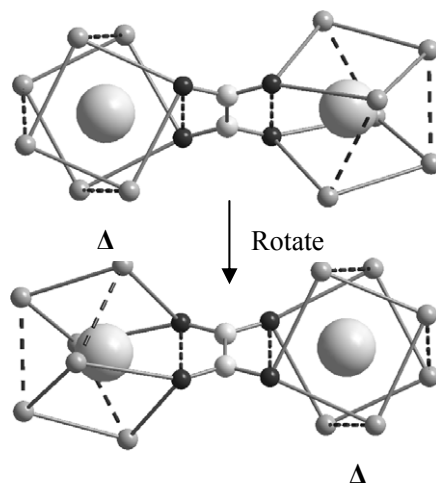


Fig. S1. Absolute coordination configuration around the Dy(III) ions.
Nomenclature of Inorganic Chemistry (IUPAC Recommendations 2005)

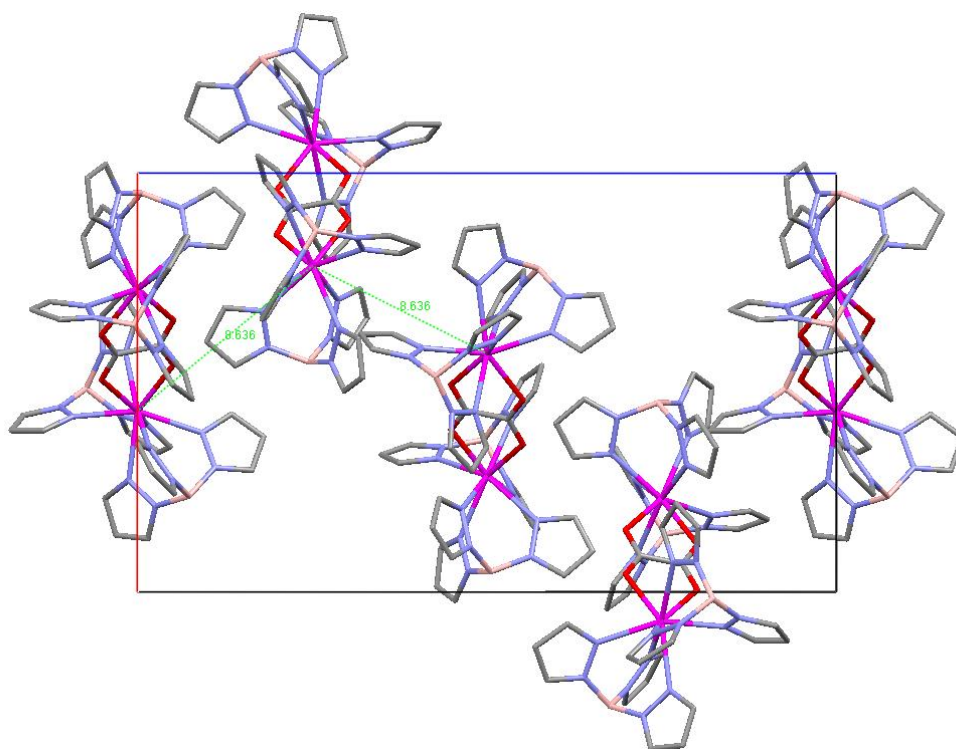


Fig. S2. Packing diagram of compound **1**, showing the shortest intermolecular Dy...Dy distance, between dinuclear [Dy₂] units.

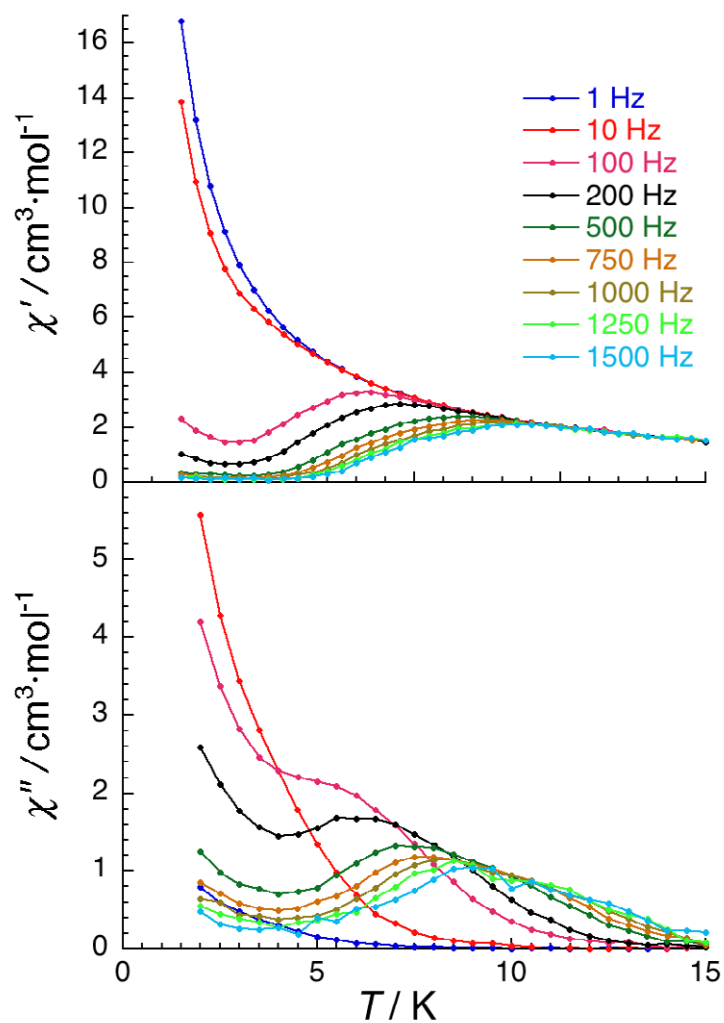


Fig. S3. Temperature dependence of the in-phase (top) and out-of-phase (bottom) ac susceptibility under zero-dc field for 1.

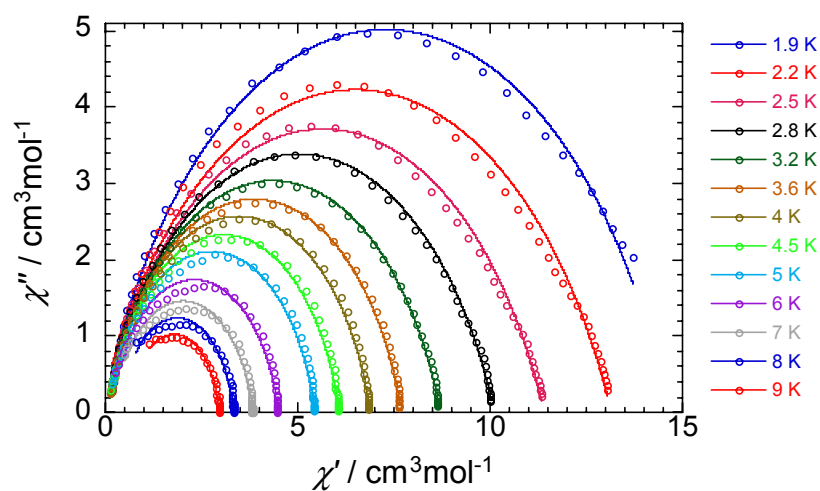


Fig. S4. Cole-Cole plots measured below 9 K and zero-dc field; the solid lines are the best fits to the experimental data, obtained with the generalized Debye model with α parameters below 0.25.

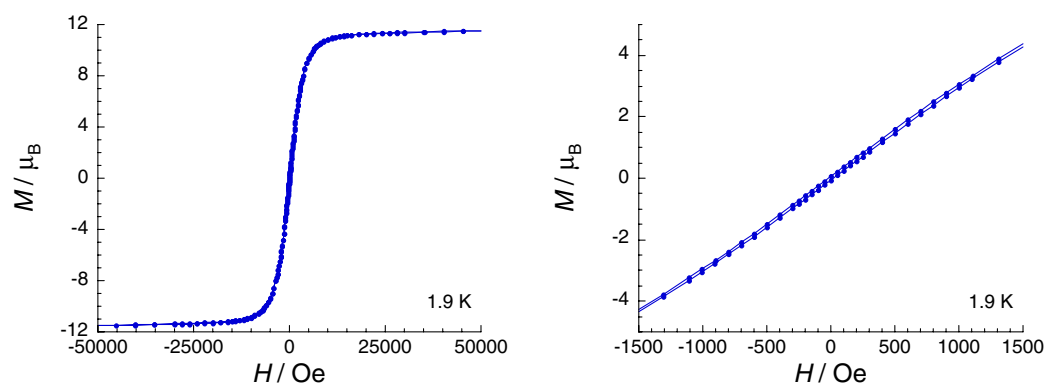


Fig. S5. M vs. H data of **1** at 1.9 K emphasizing the absence of significant magnetic hysteresis loop at 1.9 K