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A mononuclear dysprosium(III) single-molecule magnet with non-planar metallacrown

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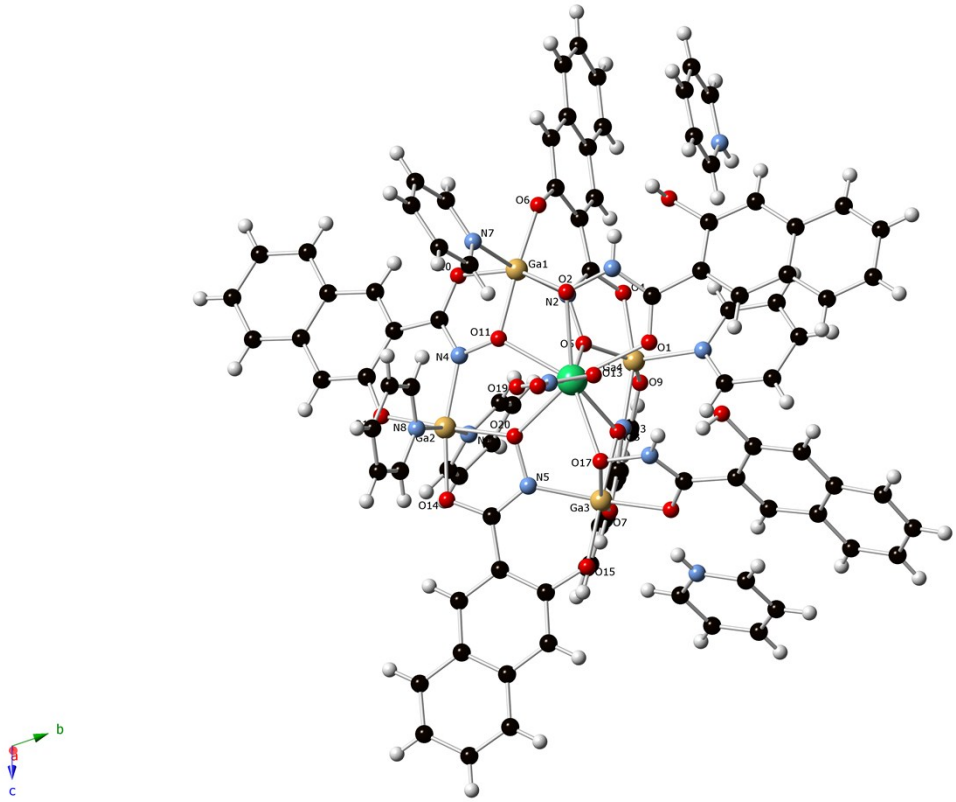

Figure S1. Molecular structure of **1** obtained from X-ray diffraction. Color code: Dy (green), O (red), N (light blue), Ga (light brown), C (grey), H (white).

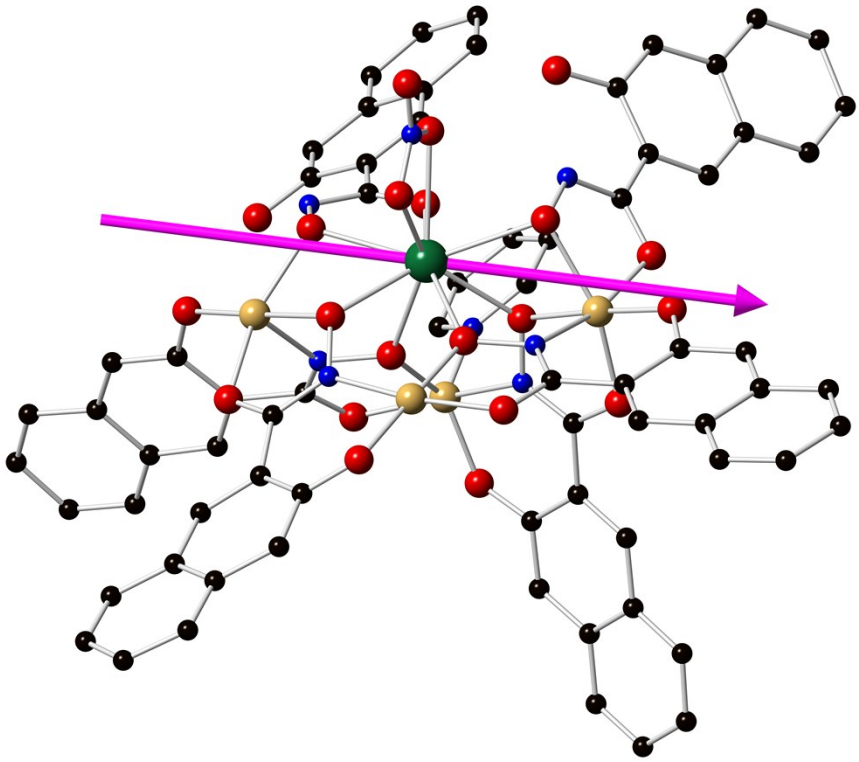

Figure S2. Molecular structure with anisotropic axis (violet arrow), the H atoms, pyridine molecules and two pyridinium cations were omitted for clarity.

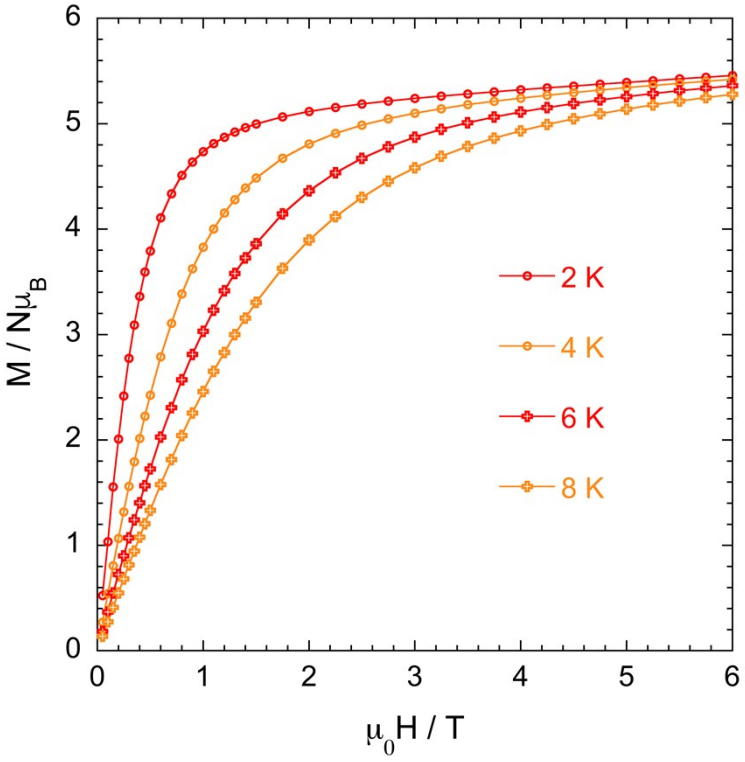

Figure S3. Magnetization *vs.* $\mu_0 H$ at variable temperatures for complex **1**.

Table S1. SHAPE analysis of night-coordinate geometry for complex **1**.

Label	EP-9	OPY-9	HPBY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	**TCTPR-9**	JTDIC-9	HH-9	MFF-9
1	34.953	22.819	15.519	13.271	8.481	6.858	3.365	2.193	3.263	**1.744**	5.472	9.956	9.569

Vertices	**Code**	**Label**	**Shape**	**Symmetry**
9	1	EP-9	Enneagon	D_{9h}
	2	OPY-9	Octagonal pyramid	C_{8v}
	3	HBPY-9	Heptagonal bipyramid	D_{7h}
	4	JTC-9	Triangular cupola (J3) = trivacant cuboctahedron	C_{3v}
	5	JCCU-9	Capped cube (Elongated square pyramid, J8)	C_{4v}
	6	CCU-9	Capped cube	C_{4v}
	7	JCSAPR-9	Capped sq. antiprism (Gyroelongated square pyramid J10)	C_{4v}
	8	CSAPR-9	Capped square antiprism	C_{4v}
	9	JTCTPR-9	Tricapped trigonal prism (J51)	D_{3h}
	10	TCTPR-9	Tricapped trigonal prism	D_{3h}
	11	JTDIC-9	Tridiminished icosahedron (J63)	C_{3v}
	12	HH-9	Hula-hoop	C_{2v}
	13	MFF-9	Muffin	C_s

Table S2. Lanthanide center bonds with oxygen for **1**.

Bond length / Å	
Dy1–O1	2.335
Dy1–O2	2.413
Dy1–O5	2.413
Dy1–O8	2.349
Dy1–O11	2.346
Dy1–O3	2.522
Dy1–O17	2.487
Dy1–O19	2.418
Dy1–O_{ave}	2.410

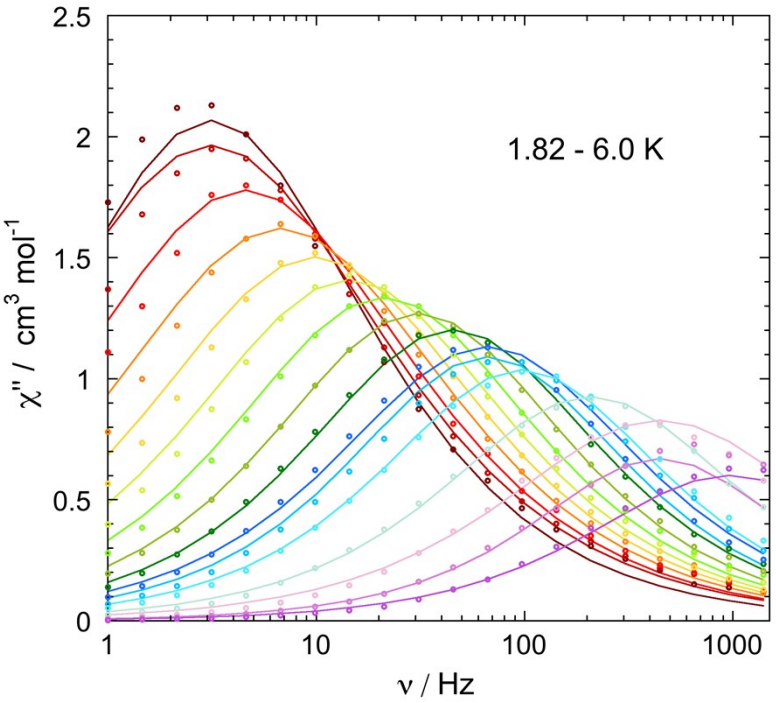

Figure S4. Frequency dependent out-of-phase ac magnetic susceptibilities (ᔓ (exp), — (fit)) for complex **1**.

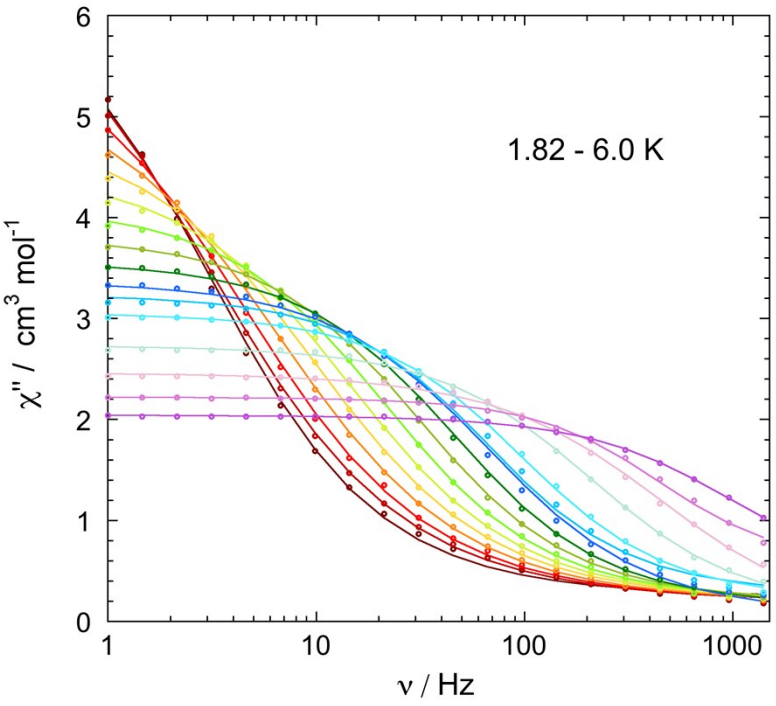

Figure S5. Frequency dependent in-phase ac magnetic susceptibilities (ᔓ (exp), — (fit)) for complex **1**.

Table S3. Cole-cole fit parameters for complex **1**.

Complex	T / K	χ_0	χ_∞	α	τ
1	1.82	6.5367793166	0.2414925008	0.2596179854	0.0506988152
	2.00	6.7228981635	0.1894825429	0.3103464591	0.0507019479
	2.20	5.9737800576	0.1967294461	0.2968456773	0.0345998152
	2.40	5.4109641789	0.1872390489	0.2925439220	0.0235951331
	2.60	4.9189901593	0.1952242819	0.2784341372	0.0160994923
	2.80	4.4924821594	0.1980955828	0.2602010414	0.0109998221
	3.00	4.1325269900	0.1975994005	0.2399391750	0.0075396453
	3.20	3.8236301172	0.1884452784	0.2227793349	0.0051498896
	3.40	3.5754830849	0.1451626183	0.2207187155	0.0035198186
	3.60	3.3775557209	0.0632941950	0.2362854596	0.0024017707
	3.80	3.2416245284	0.2699640730	0.1935040247	0.0024009947
	4.00	3.0607057822	0.2033755626	0.2006550723	0.0016403573
	4.50	2.7352971938	0.097486081	0.2200900638	0.0007659100
	5.00	2.4207579344	0.4316980088	0.1207035680	0.0005396655
	5.50	2.2221660767	0.5451752431	0.1417760770	0.0003579929
	6.00	2.0435783951	0.3839517052	0.2021980425	0.0001640466