Supplementary Information

A Nested Spin Structure and Single Molecule Magnet Behaviour in an Fe_8Dy_{12} Heterometallic Cyclic Coordination Cluster

Yan Peng,[*a,b] Jonas Braun,[a,c] Michael Schulze,[d] Hagen Kaemmerer,[a,e] Yannik F. Schneider,[a,c] Christopher E. Anson,[a] Wolfgang Wernsdorfer[d] and Annie K. Powell[*a,b,e]

[a]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), Engesserstraße 15, 76131 Karlsruhe, Germany
[b]School of Chemistry and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, P.R. China.
[c]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[d]Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[e]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Engesserstrasse 15,76131 Karlsruhe, Germany

Email: annie.powell@kit.edu, Email: py16882020@163.com

Table of Content

1. Experimental

Crystallography:

Data were measured from a crystal of dimensions 0.07 × 0.05 × 0.04 mm^3 cooled to 150(2) K on a Bruker SMART Apex diffractometer on the PDIFF beamline with silicon-monochromated radiation of λ = 0.79942 Å from the ANKA (now KARA) synchrotron, Karlsruhe. Data were corrected for polarisation effects, absorption and primary beam decay.

The structure was solved by dual-space direct methods using SHELXT[a] and refined by full-matrix least-squares using SHELXL[b] on the Olex2 platform[c]. One tea ligand was disordered by twisting about the Dy-N bond, and the three methylene groups were refined as pairs of isotropic half-occupancy C atoms with similarity restraints on their N-C and C-C bond lengths. OH H-atoms were refined with restraints on the O-H bond lengths. Some of the lattice solvent molecules could be refined anisotropically, but others were badly disordered and their contributions to the structure factors were calculated using SQUEEZE.[d]

Crystallographic and refinement parameters are summarised in Table S1. Full crystallographic data and details of the structural determinations for the structures in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2306455. Copies of the data can be obtained, free of charge, from https://www.ccdc.cam.ac.uk/structures/

Crystal data for **1:** $C_{142}H_{300}Dy_{12}Fe_8N_{40}O_{102}$, 6597.00 g mol^{-1}, tetragonal, $I4_1/acd$, a = 37.7905(13), c = 61.582(2) Å, Z = 16, V = 87947(7) $Å^3$, T = 150(2) K, ρ_{calc} = 1.993 g cm^{-3}, F(000) = 51968, λ = 0.79942 Å, μ = 6.236 mm^{-1}; 139306 data, 22903 unique (R_{int} = 0.0369), 1298 parameters, final wR_2 = 0.1996, S = 1.576 (all data), R_1 (18273 data with I > 2σ(I)) = 0.0575. Full crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre as CCDC 2306455 (https://www.ccdc.cam.ac.uk/structures/)

Materials

Elemental analyses (C/H/N) were performed using an Elemental Vario EL analyzer at the Institute of Inorganic Chemistry, Karlsruhe Institute of Technology. The IR spectrum was measured on a Nicolet iS 50 with ATR attachment. All reagents were obtained from commercial sources and used as received.

$[Fe_8Dy_{12}(tea)_8(teaH)_{12}(NO_3)_{12}]\cdot 8MeCN$ (1)

A solution of 109 mg $teaH_3$ (1 mmol) and 100 µl Et_3N in 10ml MeCN was added dropwise to a stirred solution of 101 mg $Fe(NO_3)_3\cdot 9H_2O$ (0.25 mmol) and 112 mg $Dy(NO_3)_3\cdot 6H_2O$ (0.25 mmol) in 5 ml MeOH. This mixture was left stirring for 10 minutes after which 80 µl of Et_3N were added dropwise. After another 10 minutes of stirring the glass vial was sealed and left undisturbed to allow for crystallisation. The product was isolated after 14 days as colourless block shaped crystals in a yield of 47% (based on Dy).

Elemental analysis (calculated, $C_{142}H_{300}Dy_{12}Fe_8N_{40}O_{102}$) C: 25.50%, H: 4.34%, N: 8.75%; (found) C: 25.46% H: 4.19% N: 8.62%.
ATR-IR (4000-400 cm^{-1}): 2963(w); 2849(s); 2705(w); 1628(w); 1458(s); 1366(m); 1289(s); 1163(w); 1060(s); 1023(s); 894(s); 814(m); 739(m); 621(m); 588(m); 551(m); 459(m).

Magnetic Measurements

Magnetic susceptibility measurements on polycrystalline samples were obtained using a Quantum Design SQUID magnetometer MPMS-XL in the temperature range 1.8-300 K. Magnetisation isotherms were collected at 2-10 K between 0 and 7 T. Alternating current (ac) susceptibility measurements were performed with an oscillating field of 3 Oe and ac frequencies ranging from 1 to 1500 Hz. The magnetic data were corrected for the sample holder and the diamagnetic contribution.

2. Crystallographic data

Table S1 Crystal data and structure refinement for compound (**1**)

Formula	$C_{142}H_{300}Dy_{12}Fe_8N_{40}O_{102}$
Formula weight / g mol^{-1}	6597.00
Crystal System	Tetragonal
Space Group	$I4_1/acd$
a / Å	37.7905(13)
c / Å	61.582(2)
U / Å^3	87947(7)
Z	16
T / K	150
F(000)	51968
D_c / Mg m^{-3}	1.993
λ / Å	0.79942
μ / mm^{-1}	6.236
Data Measured	139306
Unique Data	22903
R_{int}	0.0369
Data with I ≥ 2σ(I)	18273
wR_2 (all data)	0.1996
S (all data)	1.576
R_1 [I ≥ 2σ(I)]	0.0575
Parameters/Restraints	1298 / 43
Biggest diff. peak/hole / eÅ^{-3}	4.35 / -2.65
CCDC number	2306455

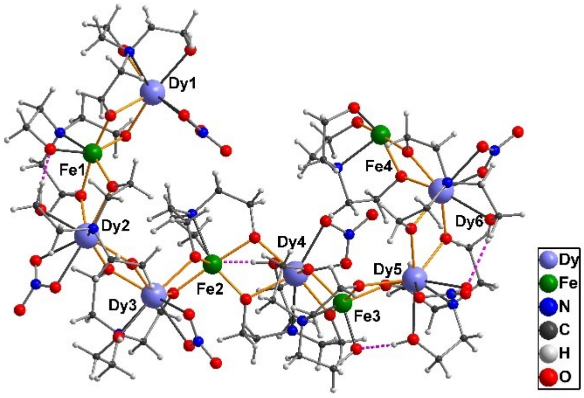


Fig. S1 Asymmetric unit of the compound (**1**).

Table S2 Selected bond length (Å) and angles (°) for compound (**1**)

Dy1—O29^{i}	2.252 (6)	Dy4—O40	2.505 (6)	Fe3—O22	1.965 (6)
Dy1—O2	2.275 (7)	Dy4—N6	2.565 (8)	Fe3—O21	1.994 (7)
Dy1—O4	2.304 (6)	Dy5—O20	2.258 (6)	Fe3—O17	2.002 (6)
Dy1—O1	2.323 (6)	Dy5—O25	2.274 (6)	Fe3—O19	2.006 (6)
Dy1—O3	2.379 (8)	Dy5—O22	2.284 (6)	Fe3—O20	2.050 (6)
Dy1—O32	2.466 (8)	Dy5—O23	2.302 (6)	Fe3—N7	2.243 (7)
Dy1—O31	2.527 (7)	Dy5—O24	2.424 (6)	Fe4—O30	1.973 (6)
Dy1—N1	2.585 (9)	Dy5—O44	2.471 (6)	Fe4—O1i	1.979 (7)
Dy2—O5	2.268 (6)	Dy5—O43	2.552 (6)	Fe4—O28	2.000 (6)
Dy2—O10	2.279 (6)	Dy5—N8	2.590 (7)	Fe4—O26	2.014 (7)
Dy2—O7	2.298 (6)	Dy6—O23	2.241 (6)	Fe4—O29	2.038 (6)
Dy2—O8	2.310 (6)	Dy6—O26	2.279 (7)	Fe4—N10	2.204 (9)
Dy2—O9	2.454 (7)	Dy6—O25	2.287 (6)	Fe1—O5—Dy2	105.0 (2)
Dy2—O35	2.480 (7)	Dy6—O28	2.289 (6)	Fe1—O7—Dy2	106.2 (3)
Dy2—O34	2.489 (7)	Dy6—O27	2.498 (8)	Dy3—O8—Dy2	109.3 (2)
Dy2—N3	2.591 (8)	Dy6—O47	2.499 (8)	Dy3—O10—Dy2	111.5 (2)
Dy3—O10	2.252 (6)	Dy6—O46	2.505 (8)	Fe2—O11—Dy3	107.2 (2)
Dy3—O8	2.280 (5)	Dy6—N9	2.575 (8)	Fe2—O13—Dy3	105.8 (2)
Dy3—O13	2.320 (5)	Fe1—O7	1.960 (6)	Fe2—O14—Dy4	102.6 (2)
Dy3—O11	2.325 (6)	Fe1—O4	1.994 (6)	Fe2—O16—Dy4	104.2 (3)
Dy3—O38	2.485 (6)	Fe1—O6	1.997 (7)	Fe3—O17—	107.6 (3)

				Dy4	
Dy3—O12	2.489 (6)	Fe1—O2	2.009 (7)	Fe3—O19—Dy4	106.8 (2)
Dy3—O37	2.489 (6)	Fe1—O5	2.027 (6)	Fe3—O20—Dy5	105.3 (2)
Dy3—N4	2.581 (7)	Fe1—N2	2.231 (8)	Fe3—O22—Dy5	107.2 (2)
Dy4—O16	2.290 (6)	Fe2—O16	1.987 (6)	Dy6—O23—Dy5	111.0 (3)
Dy4—O14	2.292 (6)	Fe2—O11	1.991 (6)	Dy5—O25—Dy6	110.3 (2)
Dy4—O17	2.294 (6)	Fe2—O15	2.000 (6)	Fe4—O26—Dy6	106.4 (3)
Dy4—O19	2.311 (5)	Fe2—O14	2.035 (6)	Fe4—O28—Dy6	106.5 (3)
Dy4—O18	2.395 (6)	Fe2—O13	2.036 (5)	Fe4—O29—Dy1i	104.0 (3)
Dy4—O41	2.443 (6)	Fe2—N5	2.195 (7)		

Table S3 SHAPE analysis of compound (**1**) and reported {$Fe_{10}Dy_{10}$}

	Fe10Dy10-Rac	Fe8Dy12
Fe1	OC 2.96 TRP 9.44	OC 3.52 TRP 8.06
Fe2	OC 2.68 TRP 9.57	OC 2.33 TRP 9.57
Fe3	OC 2.90 TRP 9.32	OC 3.38 TRP 8.22
Fe4	OC 3.18 TRP 9.40	OC 2.40 TRP 9.50
Fe5	OC 2.45 TRP 9.33	-
Dy1	TDD 2.65 JBTPR 3.40 BTPR 2.99	TDD 2.84 JBTPR 3.44 BTPR 3.16
Dy2	TDD 2.71 JBTPR 3.04 BTPR 2.51	TDD 2.76 JBTPR 3.57 BTPR 2.31
Dy3	TDD 2.56 JBTPR 3.23 BTPR 2.71	TDD 2. 39 JBTPR 3.57 BTPR 3.35
Dy4	TDD 2.64	TDD 2.68

	JBTPR 3.45 BTPR 2.98	JBTPR 3.50 BTPR 3.24
Dy5	TDD 2.69 JBTPR 3.89 BTPR 3.53	TDD 2.29 JBTPR 2.34 BTPR 2.15
Dy6	-	TDD 3.05 JBTPR 3.08 BTPR 2.54

OC, octahedron; TPR, trigonal prismatic; TDD, Triangular dodecahedron; JBTPR, Biaugmented trigonal prism J50; BTPR, Biaugmented trigonal prism.

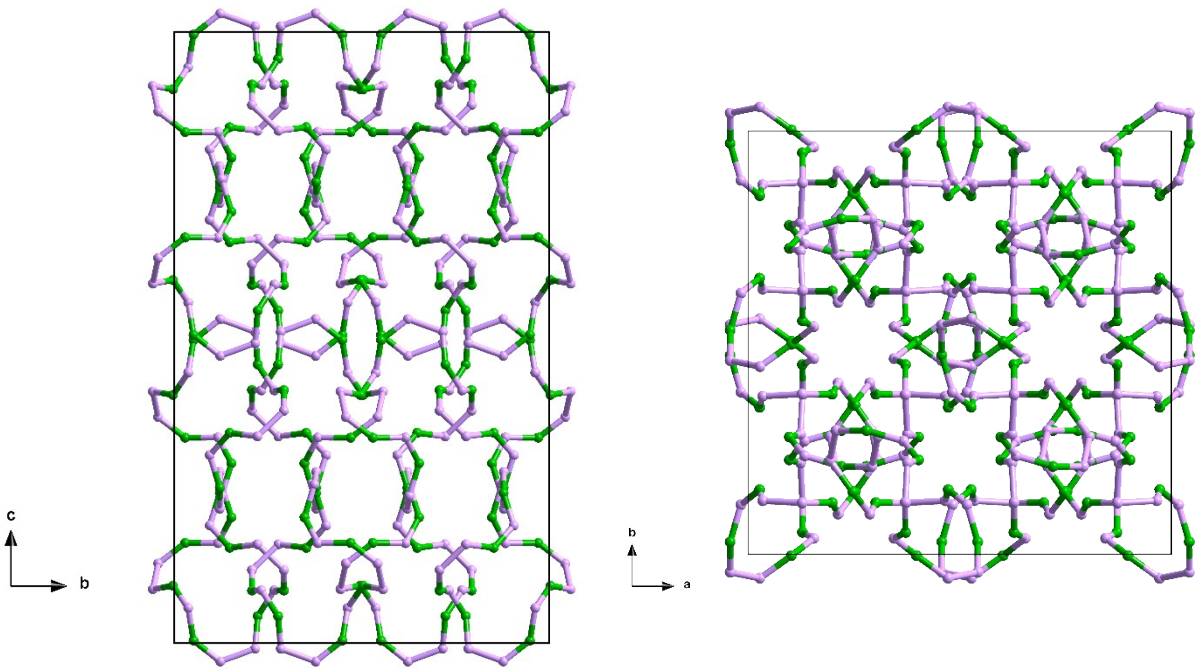


Fig. S2 Crystal packing of compound (**1**). Ligands omitted for clarity

3. Magnetic Data

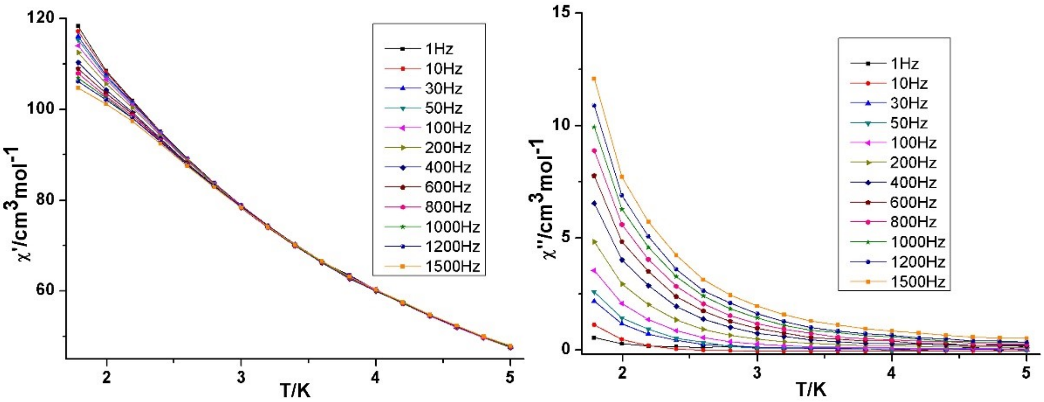


Fig. S3 Plots of χ' (left) and χ'' (right) vs temperature at different frequencies for (**1**).

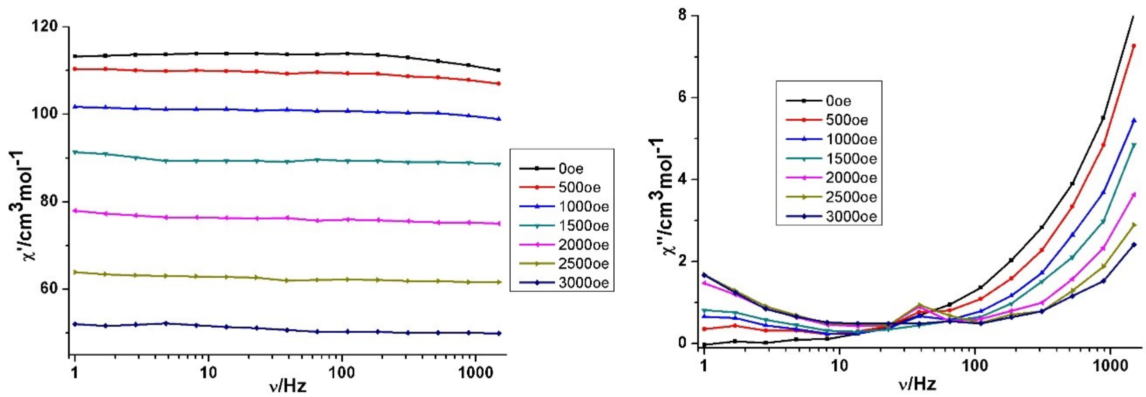
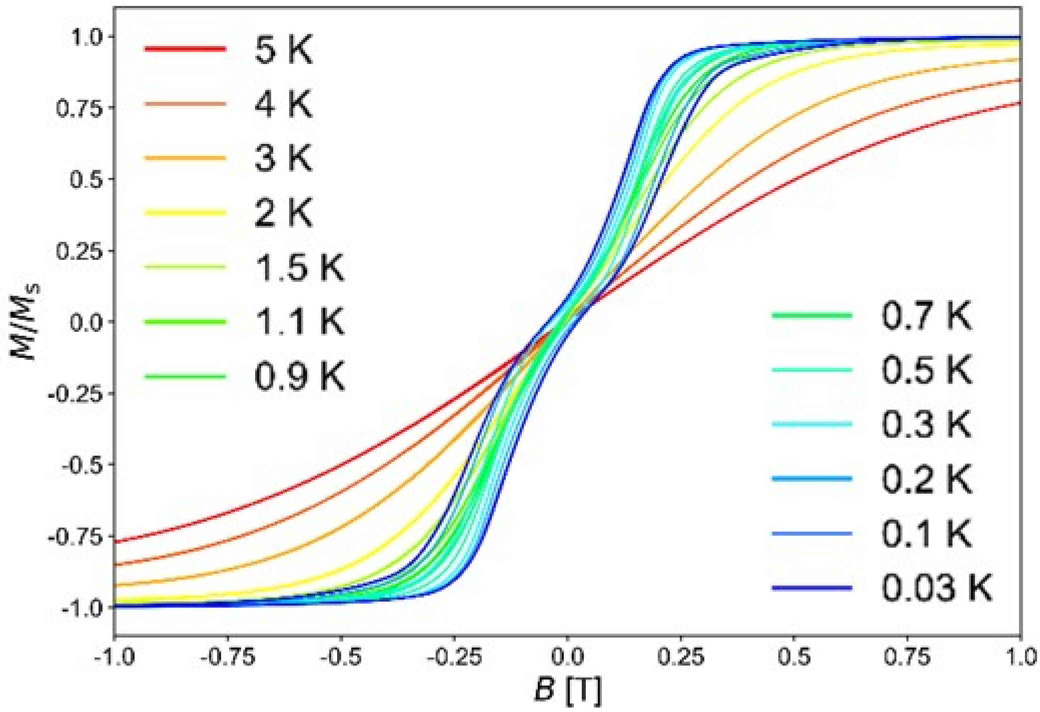


Fig. S4 Plots of χ' (left) and χ'' (right) vs frequency under different dc magnetic fields for (**1**) at 1.8 K



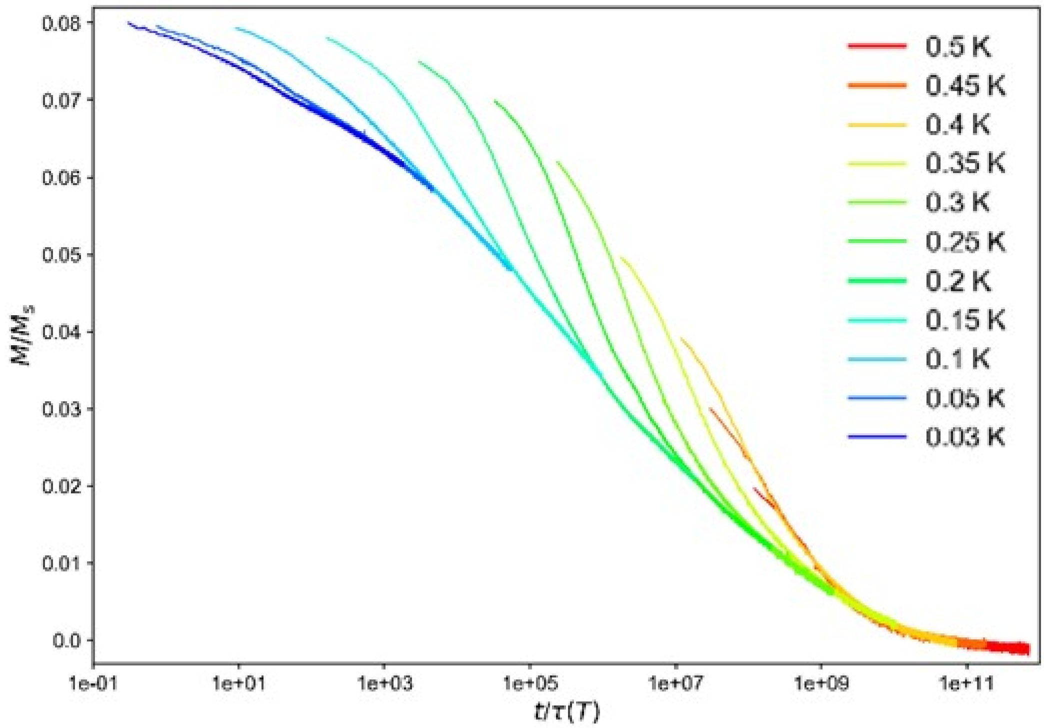


Fig. S5. Temperature-dependent microSQUID measurements (top) and magnetisation decay at low temperatures (bottom).

4. MAGELLAN

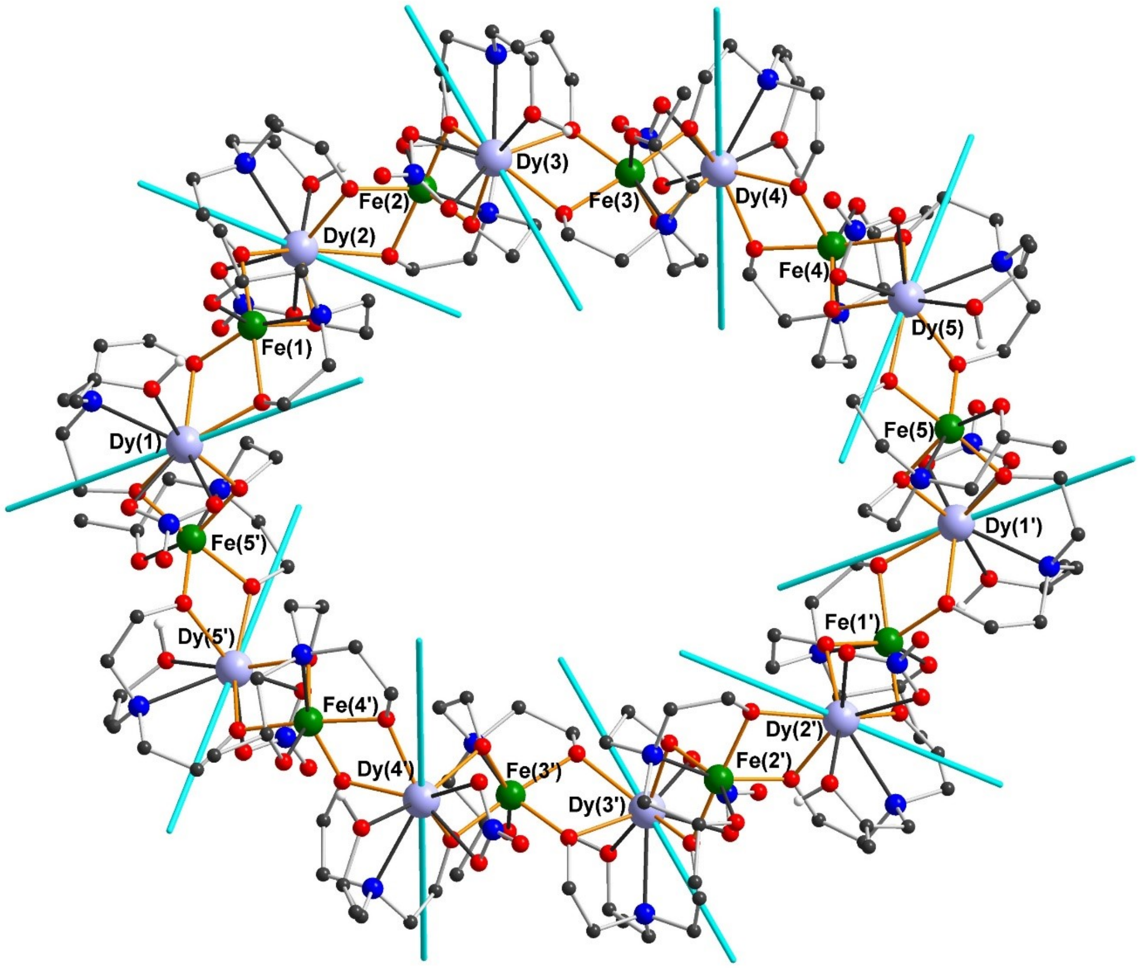


Fig. S6. Arrangement of the anisotropy axes in $Fe_{10}Dy_{10}$ calculated using MAGELLAN.[e]

For the MAGELLAN analysis of compound (**1**) Fe_8Dy_{12} **t**he charges have been assigned as described in the original publication on MAGELLAN.[e] In the case for compound (**1**) this means Fe and Dy all as +3, alkoxo oxygens as -1, nitrate nitrogens as +1, nitrate oxygens as -0.6667 and all other atoms neutral.

MAGELLAN output file for compound (1):

fe8dy12.xyz; Generated by MAGELLAN, (C) 2013 NICHOLAS F CHILTON and ALESSANDRO SONCINI, nfchilton@gmail.com, asoncini@unimelb.edu.au

Dy1 19.55054 14.47716 20.72422

Be1a	14.69398	13.60332	19.91786
Be1b	24.40710	15.35100	21.53058
Dy2	20.50248	20.49492	22.77121
Be2a	21.83224	19.02076	27.36017
Be2b	19.17272	21.96908	18.18225
Dy3	17.84694	21.03646	25.35643
Be3a	22.19971	19.17171	26.96146
Be3b	13.49417	22.90121	23.75140
Dy4	13.03546	17.47357	27.24762
Be4a	10.33703	19.34091	31.02009
Be4b	15.73389	15.60623	23.47515
Dy5	14.03539	14.25080	32.63974
Be5a	18.20765	17.00610	32.66383
Be5b	9.86313	11.49550	32.61565
Dy6	14.22850	10.74044	31.35391
Be6a	18.30061	8.17070	30.00691
Be6b	10.15639	13.31018	32.70091
Dy1'	13.86571	8.79234	25.46235
Be1a'	12.99188	3.93578	24.65595
Be1b'	14.73954	13.64890	26.26875
Dy2'	7.84795	7.84040	23.41536

Be2a'	6.37380	9.17016	28.00433
Be2b'	9.32210	6.51064	18.82639
Dy3'	7.30642	10.49593	20.83015
Be3a'	5.44167	14.84870	22.43518
Be3b'	9.17117	6.14316	19.22512
Dy4'	10.86930	15.30742	18.93896
Be4a'	12.73659	12.60899	22.71146
Be4b'	9.00201	18.00585	15.16646
Dy5'	14.09208	14.30748	13.54683
Be5a'	16.84736	18.47975	13.57092
Be5b'	11.33680	10.13521	13.52274
Dy6'	17.60244	14.11437	14.83266
Be6a'	20.17222	10.04230	16.17968
Be6b'	15.03266	18.18644	13.48564
Fe1	20.50021	17.78383	20.70021
Fe2	15.03571	19.01807	25.00418
Fe3	14.05391	16.94450	30.52255
Fe4	15.21786	10.47099	28.06912
Fe1'	10.55904	7.84266	25.48637
Fe2'	9.32481	13.30717	21.18239
Fe3'	11.39837	14.28897	15.66402

Fe4'	17.87188	13.12502	18.11745
N	21.81872	13.43414	20.05236
C	22.03451	13.81507	18.63351
C	20.81727	13.46324	17.80893
O	19.62839	13.97153	18.45800
C	22.83415	14.08301	20.89665
C	22.66712	15.56969	20.90589
O	21.28814	15.94117	20.84246
C	21.82855	11.98034	20.20078
C	20.86376	11.54802	21.18794
O	19.53089	12.11374	20.99888
H	19.20702	11.79819	20.13488
N	20.02292	18.24865	18.57131
C	18.88731	17.40253	18.19074
C	18.03892	17.09982	19.36942
O	18.87447	16.66032	20.43109
C	19.78408	19.72966	18.47340
C	19.04603	20.19978	19.72475
O	19.64312	19.61327	20.86648
C	21.30704	17.93197	17.87482
C	22.49631	18.54342	18.68339

O	22.25407	18.46671	20.03389
N	22.56735	19.67751	24.10693
C	22.72116	18.22409	23.98007
C	21.38716	17.52345	23.64876
O	20.70806	18.21275	22.60125
C	22.32171	20.14498	25.50053
C	20.90986	19.77728	25.95378
O	19.93638	20.19940	24.99186
C	23.74188	20.41556	23.56993
C	23.85790	20.30295	22.02545
O	22.56924	20.48699	21.44781
H	22.40825	19.93033	20.66326
N	16.90029	23.30691	24.57618
C	17.24116	23.45694	23.09144
C	17.54084	22.17509	22.43805
O	18.43610	21.35277	23.20598
C	15.40983	23.20639	24.73014
C	14.84562	21.95401	24.16974
O	15.65018	20.87056	24.61252
C	17.41348	24.39641	25.39153
C	18.92548	24.29551	25.56150

O	19.21269	22.99741	26.05292
H	20.10266	23.19770	26.10773
N	15.60105	17.93537	23.18073
C	17.09302	18.02418	23.09144
C	17.62662	17.88549	24.52261
O	17.03671	18.86275	25.34658
C	15.12414	16.54581	23.27988
C	14.35019	16.25634	24.47149
O	14.51458	17.12325	25.53255
C	14.89286	18.67682	22.09135
C	13.43150	18.84990	22.52365
O	13.37179	19.24066	23.91664
N	11.54084	19.52408	27.62080
C	12.48447	20.67480	27.98599
C	13.64691	20.65440	27.14601
O	14.18731	19.39220	26.76112
C	10.74195	19.24028	28.87030
C	11.50607	18.59784	29.91289
O	12.62089	17.86433	29.46950
C	10.67317	19.90086	26.43473
C	10.48271	18.76752	25.52393

O	11.69049	17.99168	25.33488
H	12.05252	18.60464	24.66302
N	15.91282	18.19877	30.57921
C	16.40410	18.30118	29.15912
C	16.07835	17.00232	28.41521
O	14.70731	16.69660	28.64183
C	16.90369	17.53782	31.49309
C	16.73099	16.05265	31.57006
O	15.34861	15.69780	31.50910
C	15.43780	19.45946	31.12606
C	14.55577	19.20098	32.31213
O	13.70813	18.10165	32.10952
N	11.52837	14.45713	33.25680
C	10.80922	15.21030	32.19020
C	11.52346	15.17591	30.82677
O	12.93115	15.40719	31.00843
C	11.01177	13.08080	33.40952
C	11.45166	12.21238	32.22468
O	12.84990	12.37979	32.01222
C	11.44750	15.19556	34.53647
C	12.23808	16.46608	34.52293

O	13.51577	16.26616	33.88309
H	13.47382	16.80506	33.07698
N	16.28771	9.89393	32.64713
C	17.06392	11.09453	33.05419
C	16.82849	12.31668	32.17049
O	15.43251	12.55400	32.05410
C	16.94035	8.97411	31.72648
C	17.09982	9.56289	30.36059
O	15.90300	10.13088	29.93260
C	15.88108	9.11658	33.82828
C	14.85507	9.84102	34.63747
O	13.81999	10.37047	33.79071
H	13.59740	11.09567	34.35296
N	15.93361	12.51697	27.67007
C	15.21181	13.39258	28.61474
C	13.79958	12.85482	28.86415
O	13.89443	11.45052	29.20408
C	15.62448	12.84688	26.26784
C	14.39062	12.15342	25.77149
O	14.33016	10.84096	26.27216
C	17.39119	12.36543	27.90223

C	17.92441	11.09491	27.21744
O	16.99401	10.05719	27.31536
N	19.14316	14.39365	23.61550
O	20.29539	14.15405	23.11730
O	18.22787	14.64798	22.79831
O	18.97952	14.42652	24.82374
N	20.87396	23.32808	22.43744
O	20.48132	22.61648	21.46875
O	21.34218	22.72607	23.45354
O	20.76890	24.54984	22.41342
N	17.64552	21.30439	28.25879
O	16.77483	21.81532	27.46377
O	18.52641	20.57390	27.70086
O	17.61755	21.48201	29.45164
N	11.44485	15.07010	27.17988
O	10.92712	16.16602	27.59740
O	12.62618	15.12262	26.72294
O	10.81829	14.03501	27.19773
N	15.21823	13.50028	35.17816
O	15.82175	14.35283	34.45888
O	14.03879	13.15298	34.85301

O	15.78660	12.92662	36.09081
N	12.67796	8.29237	31.29787
O	13.89746	8.26365	31.53373
O	12.11790	9.42419	31.11559
O	12.01738	7.23612	31.19195
N	14.90873	6.52415	26.13421
C	14.52780	6.30837	27.55306
C	14.87963	7.52560	28.37765
O	14.37135	8.71449	27.72857
C	14.25987	5.50872	25.28992
C	12.77319	5.67576	25.28068
O	12.40171	7.05473	25.34411
C	16.36253	6.51433	25.98580
C	16.79485	7.47912	24.99864
O	16.22913	8.81199	25.18769
H	16.54468	9.13585	26.05169
N	10.09422	8.31996	27.61526
C	10.94035	9.45556	27.99584
C	11.24305	10.30396	26.81716
O	11.68256	9.46841	25.75548
C	8.61321	8.55879	27.71318

C	8.14310	9.29684	26.46183
O	8.72961	8.69975	25.32010
C	10.41090	7.03584	28.31175
C	9.79945	5.84657	27.50318
O	9.87617	6.08881	26.15269
N	8.66536	5.77552	22.07965
C	10.11878	5.62171	22.20651
C	10.81942	6.95572	22.53782
O	10.13012	7.63481	23.58533
C	8.19789	6.02116	20.68604
C	8.56559	7.43301	20.23280
O	8.14347	8.40650	21.19471
C	7.92731	4.60099	22.61664
C	8.03993	4.48498	24.16112
O	7.85589	5.77363	24.73876
H	8.41254	5.93462	25.52332
N	5.03596	11.44259	21.61039
C	4.88593	11.10172	23.09513
C	6.16779	10.80204	23.74852
O	6.99011	9.90678	22.98059
C	5.13648	12.93304	21.45644

C	6.38886	13.49725	22.01683
O	7.47232	12.69270	21.57406
C	3.94646	10.92939	20.79504
C	4.04736	9.41739	20.62508
O	5.34547	9.13018	20.13365
H	5.14518	8.24022	20.07884
N	10.40750	12.74182	23.00584
C	10.31870	11.24985	23.09513
C	10.45739	10.71625	21.66397
O	9.48012	11.30616	20.84000
C	11.79706	13.21874	22.90669
C	12.08654	13.99269	21.71508
O	11.21962	13.82830	20.65402
C	9.66605	13.45002	24.09523
C	9.49297	14.91138	23.66292
O	9.10222	14.97108	22.26993
N	8.81879	16.80203	18.56577
C	7.66807	15.85841	18.20059
C	7.68848	14.69597	19.04057
O	8.95068	14.15557	19.42546
C	9.10260	17.60093	17.31627

C	9.74504	16.83680	16.27369
O	10.47855	15.72198	16.71708
C	8.44202	17.66970	19.75184
C	9.57536	17.86017	20.66264
O	10.35120	16.65238	20.85170
H	9.73823	16.29035	21.52356
N	10.14410	12.43005	15.60737
C	10.04169	11.93877	17.02745
C	11.34055	12.26453	17.77136
O	11.64628	13.63557	17.54474
C	10.80506	11.43918	14.69349
C	12.29023	11.61189	14.61651
O	12.64508	12.99426	14.67748
C	8.88341	12.90508	15.06052
C	9.14190	13.78711	13.87445
O	10.24123	14.63475	14.07705
N	13.88574	16.81451	12.92978
C	13.13258	17.53366	13.99638
C	13.16697	16.81942	15.35981
O	12.93569	15.41172	15.17814
C	15.26207	17.33110	12.77705

C	16.13050	16.89122	13.96189
O	15.96309	15.49297	14.17435
C	13.14731	16.89538	11.65010
C	11.87680	16.10480	11.66365
O	12.07671	14.82710	12.30349
H	11.53782	14.86905	13.10960
N	18.44894	12.05517	13.53944
C	17.24834	11.27895	13.13238
C	16.02620	11.51439	14.01609
O	15.78887	12.91037	14.13248
C	19.36876	11.40253	14.46009
C	18.77999	11.24305	15.82598
O	18.21200	12.43988	16.25398
C	19.22629	12.46180	12.35830
C	18.50185	13.48781	11.54911
O	17.97241	14.52289	12.39586
H	17.24721	14.74548	11.83362
N	15.82591	12.40927	18.51651
C	14.95030	13.13107	17.57184
C	15.48806	14.54330	17.32243
O	16.89235	14.44844	16.98250

C	15.49599	12.71839	19.91873
C	16.18945	13.95225	20.41508
O	17.50191	14.01272	19.91442
C	15.97745	10.95169	18.28434
C	17.24796	10.41846	18.96913
O	18.28569	11.34887	18.87122
N	13.94923	9.19972	22.57107
O	14.18882	8.04749	23.06927
O	13.69490	10.11501	23.38827
O	13.91635	9.36335	21.36283
N	5.01480	7.46891	23.74914
O	5.72639	7.86156	24.71782
O	5.61680	7.00069	22.73303
O	3.79303	7.57397	23.77315
N	7.03848	10.69736	17.92778
O	6.52755	11.56805	18.72281
O	7.76897	9.81646	18.48571
O	6.86087	10.72532	16.73494
N	13.27278	16.89802	19.00670
O	12.17685	17.41575	18.58917
O	13.22025	15.71669	19.46364

O	14.30786	17.52459	18.98884
N	14.84260	13.12464	11.00842
O	13.99004	12.52113	11.72770
O	15.18989	14.30408	11.33357
O	15.41626	12.55627	10.09577
N	20.05051	15.66492	14.88870
O	20.07923	14.44542	14.65284
O	18.91868	16.22497	15.07099
O	21.10675	16.32550	14.99463

4. References

[a] G. M. Sheldrick, *Acta Cryst. A* **2015,** *71*, 3-8.

[b] G. M. Sheldrick, *Acta Cryst C* **2015**, *71*, 3-8.

[c] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009,** *42*, 339-341.

[d] A. L. Spek, *Acta Cryst C*, **2015**, *71*, 9-18.

[e] N. F. Chilton, D. Collison, E. J. McInnes, R. E. Winpenny, A. Soncini, *Nat. Commun.* **2013**, *4*, 2551.