Supporting information

Four mononuclear dysprosium complexes with neutral Schiff-base ligands: syntheses, crystal structures and slow magnetic relaxation behavior

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Computational details

Complete-active-space self-consistent field (CASSCF) calculations for **1Dy**-**4Dy** on the basis of single-crystal X-ray determined geometries have been carried out with MOLCAS 8.4 program package [1-2].

The basis sets for all atoms are atomic natural orbitals from the MOLCAS ANO-RCC library: ANO-RCC-VTZP for Dy^{3+} ion; VTZ for close O; VDZ for distant atoms. The calculations employed the second order Douglas-Kroll-Hess Hamiltonian, where scalar relativistic contractions were taken into account in the basis set and the spin-orbit couplings were handled separately in the restricted active space state interaction (RASSI-SO) procedure. For both complexes, active electrons in 7 active spaces include all f electrons (CAS(9 in 7)) in the CASSCF calculation. To exclude all the doubts, we calculated all the roots in the active space. We have mixed the maximum number of spin-free state which was possible with our hardware (all from 21 sextets, 128 from 224 quartets, 130 from 490 doublets). SINGLE_ANISO[3-5] program was used to obtain energy levels, *g* tensors, m_J values, magnetic axes, et al., based on the above CASSCF/RASSI-SO calculations.

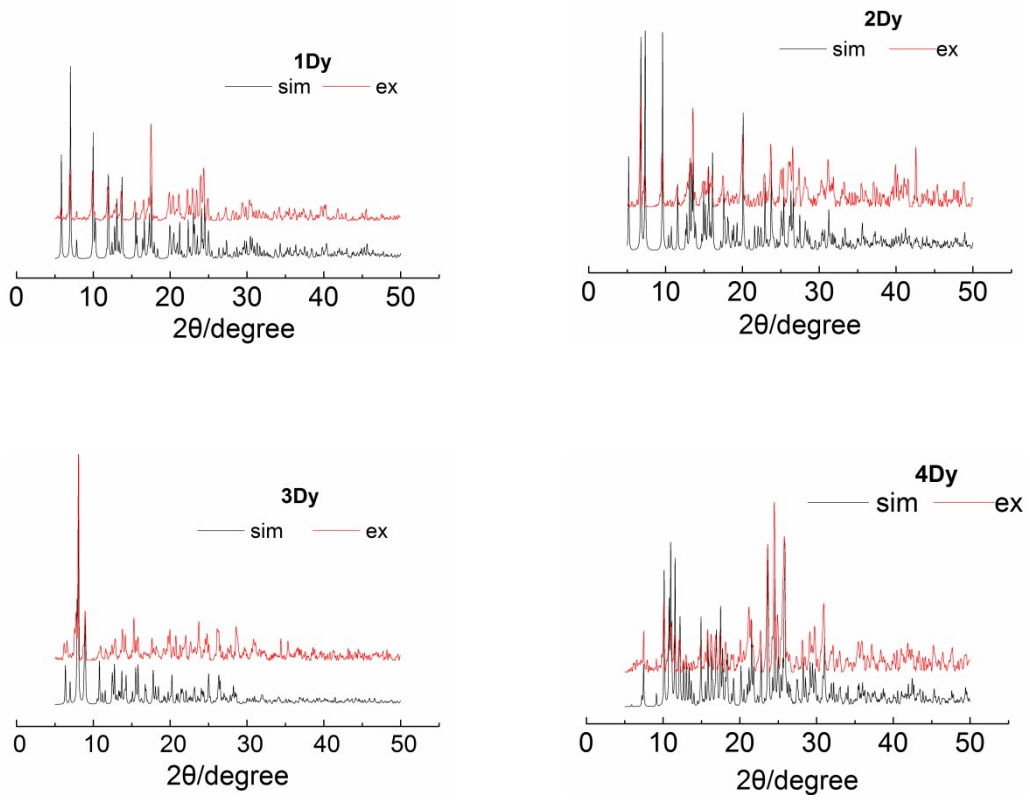

Fig. S1 Powder XRD pattern for complexes **1Dy**-**4Dy**.

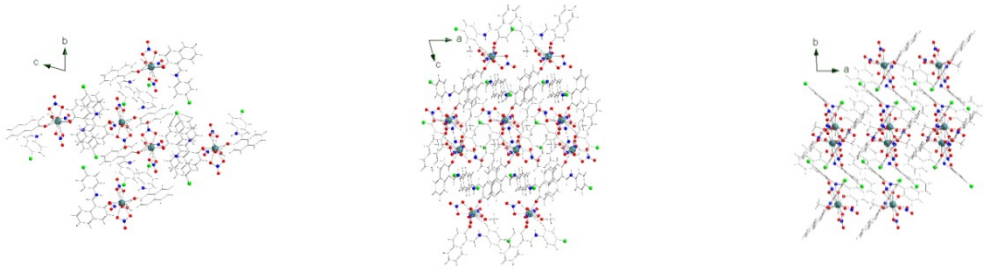

Fig. S2 Perspective view of the packing of **1Dy** along the a (left), b (center) and c (right) axes.

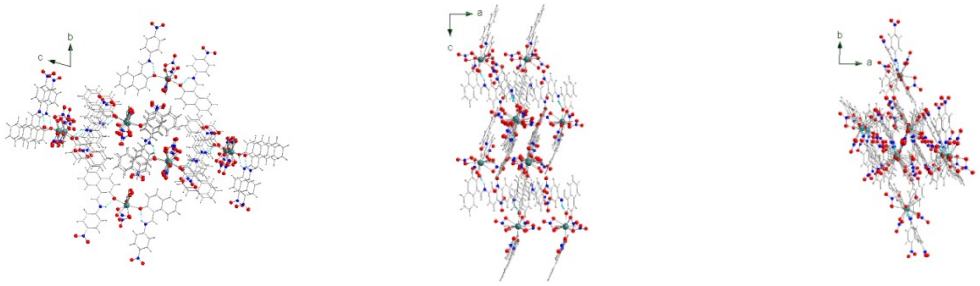

Fig. S3 Perspective view of the packing of **2Dy** along the a (left), b (center) and c (right) axes.

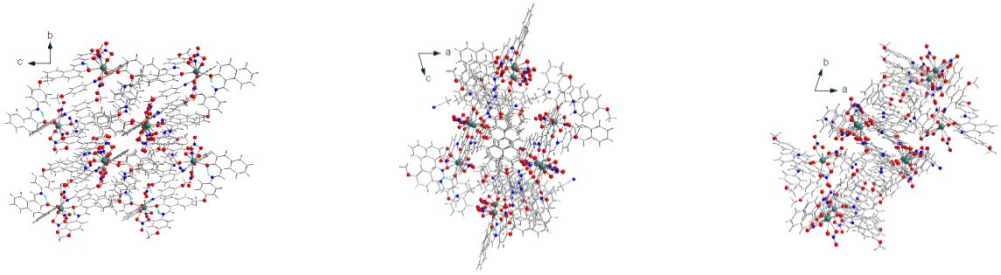

Fig. S4 Perspective view of the packing of **3Dy** along the a (left), b (center) and c (right) axes.

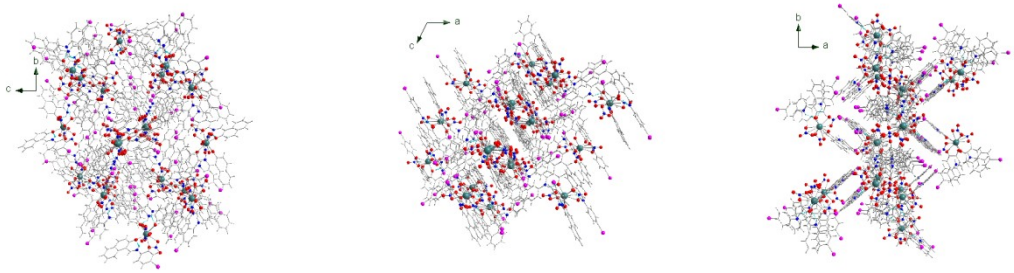

Fig. S5 Perspective view of the packing of **4Dy** along the a (left), b (center) and c (right) axes.

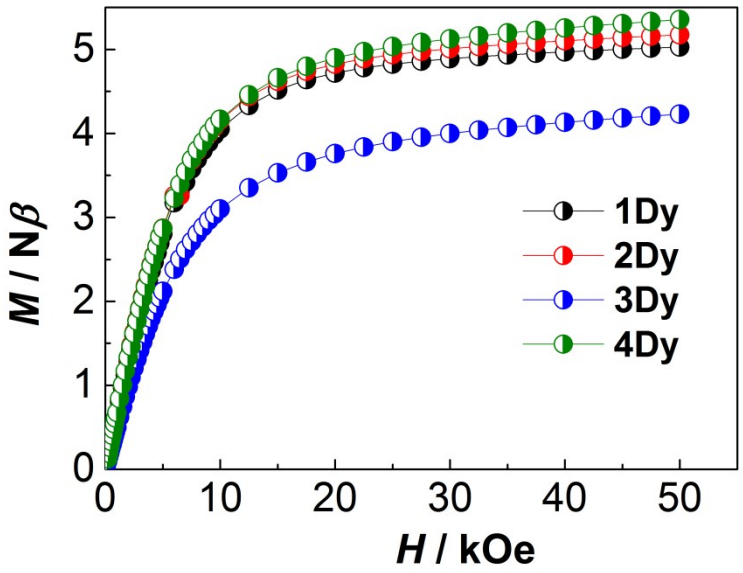

Fig. S6 *M* vs. *H* plot at 3K for complexes **1Dy-4Dy.**

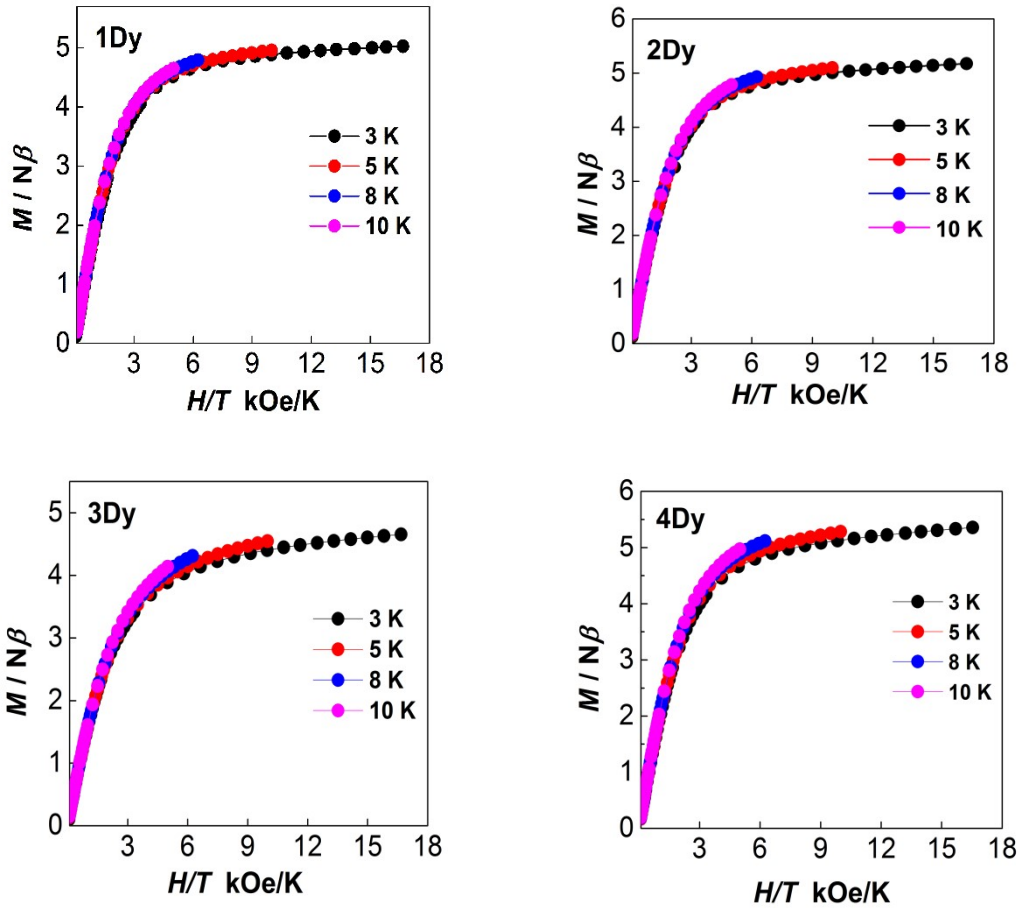

Fig.S7 *M* vs. *H/T* plot at various temperatures for complexes **1Dy-4Dy.**

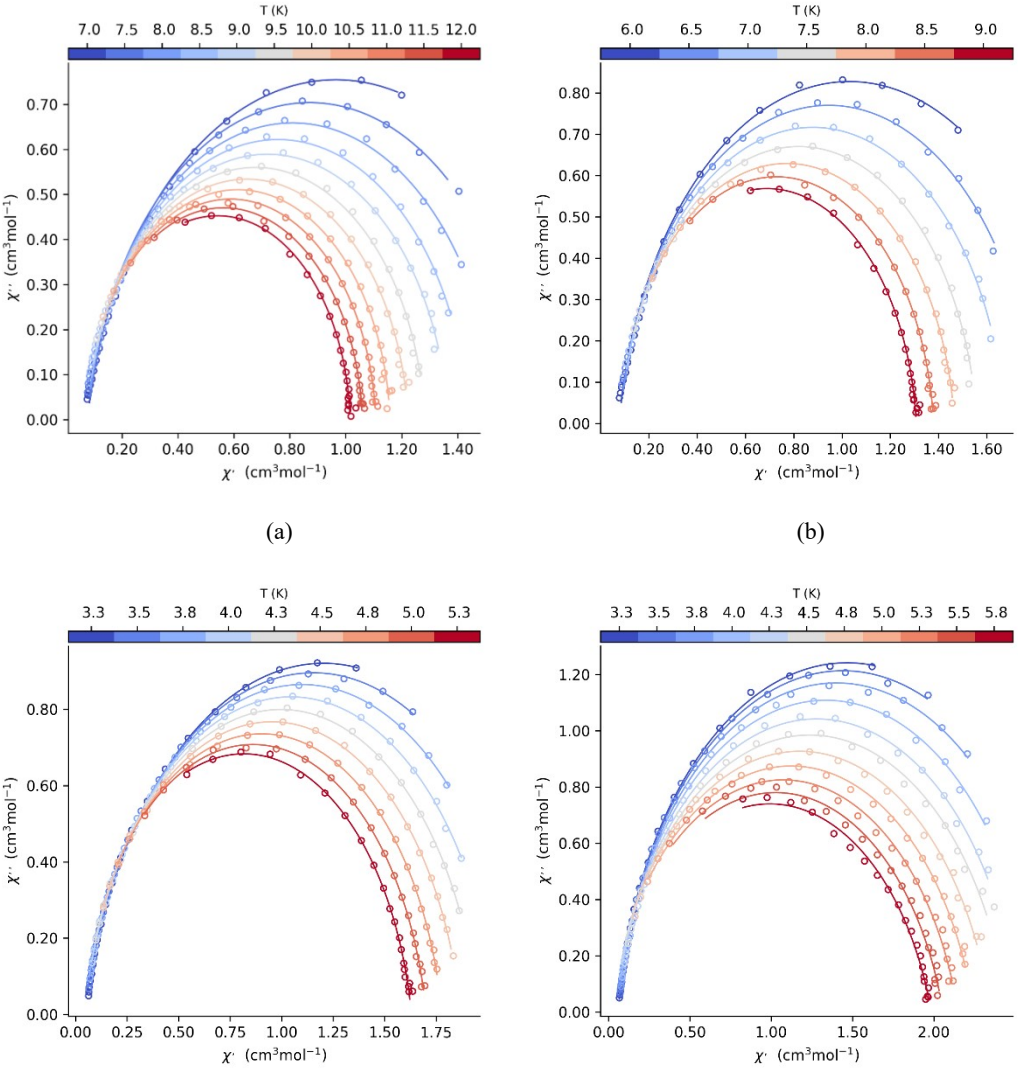

Fig. S8 Cole-Cole plots for ac-susceptibilities of complexes **1Dy**(a), **2Dy**(b), **3Dy**(c) and **4Dy**(d). The solid lines are best fits to the generalized Debye model by using CC-Fit2 program[6].

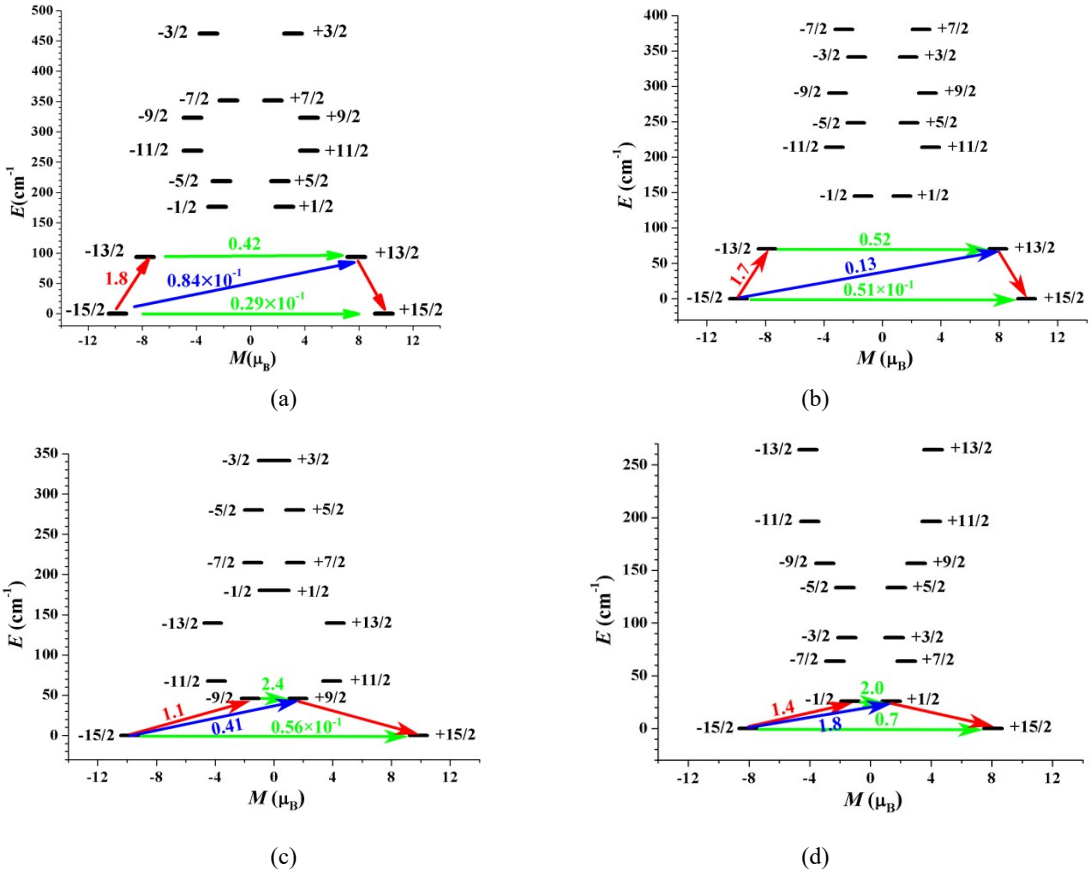

Fig. S9 Magnetization blocking barriers in four complexes **1Dy** (a), **2Dy** (b), **3Dy** (c), **4Dy** (d). The black lines represent the KDs as a function of their magnetic moments along the magnetic axis. The green lines correspond to diagonal quantum tunneling of magnetization (QTM); the blue lines represent Orbach relaxation processes. The path shown by the red arrows represents the most possible path for magnetic relaxation in the corresponding compounds. The number at each arrow is the mean absolute value of the corresponding matrix element of transition magnetic moment.

Table S1 Magnetic relaxation parameters of some Schiff-base ligated Ln-SIMs.

Complex	H_{dc} (Oe)	U_{eff}	τ_0 (s)	Ref
$[Dy(FTA)_3L]$	0	54.4 K	8.7×10^{-6}	7
$DyCl_3(N_5)\cdot 4H_2O$	0	4.13 K; 23.7 K	2.8×10^{-5}; 6.42×10^{-6}	8
$DyCl_3(N_3O_2)\cdot 6H_2O$	0	7.75 K	7.52×10^{-7}	8
$DyCl_3(db\text{-}N_3O_3)\cdot 6H_2O$	0	16.5 K	8.84×10^{-6}	8
$[Dy(TTA)_2L]$	0	67.8 K	1.2×10^{-7}	9
$[(L^{CO})Dy(N^*)_2]$	0	190 K	1.7×10^{-7}	10
$[Dy(L_1)_2(THF)_2][B(Ph)_4]$	0	263±8 cm^{-1}	5×10^{-8}	11
$[Dy(L_2)_2(py)_2][B(C_6H_5)_4]$	0	270±8 cm^{-1}	1.5×10^{-8}	11
$[Dy(NAS)_2(H_2O)_6](NAS)\cdot 3H_2O$	0	53 K	4.3×10^{-9}	12
$[Dy(hni)_2(H_2O)_2]\cdot NO_3\cdot EtOH$	0	19 K	3.8×10^{-7}	13
$[Dy(hni)(NO_3)(DMF)_2]\cdot DMF$	400	34 K	3.6×10^{-7}	13
$[Dy(NO_3)_3(salanH)_2(H_2O)]\cdot MeCN$	1000	13.1 cm^{-1}	4.5×10^{-7}	14
$[Dy(NO_3)_3(salanH)_2(MeOH)]$	1000	31 cm^{-1}	2.5×10^{-7}	14
$[K(TBPP)Dy(L)(CH_3CN)_2]$	2000	34.67 cm^{-1}	8.1×10^{-7}	15
$[DyH(TBPP)_2]$	2000	68.01 cm^{-1}	5.1×10^{-7}	15
$[Dy(H_2L)(NO_3)(H_2O)(EtOH)](NO_3)_2\cdot H_2O$	1000	20.63 K	2.69×10^{-7}	16
$[Dy(L)(NO_3)(MeOH)_2]$	1000	57.52 K; 28.49 K	1.53×10^{-12}; 6.22×10^{-7}	16
$[Dy(HL^{OCH3})(L^{OCH3})]$	300	70 K	2.2×10^{-11}	17
$[Dy(H_2dapsc)(H_2O)_4](NO_3)_3$	1000	18 K	2.67×10^{-8}	18
$[Dy(H_2L)(NO_3)_3]\ _2CH_3OH$	1000	8.8 K; 32.0 K	2.4×10^{-5}; 1.3×10^{-7}	19
$[Dy(bpdc)(Hbpdc)]\cdot 3H_2O$	2000	45.6 K	9.6×10^{-10}	20
$[Dy(12\text{-}crown\text{-}4)(NO_3)_3]$	500	75.92 K	6.8×10^{-11}	21
$[Dy(hmb)(NO_3)_2(DMF)_2]$	1800	34.1	3.2×10^{-6}	22
$[Dy(H_3L)_2](NO_3)\cdot(EtOH)\cdot 8(H_2O)$	200	60.4 K (diluted)	4.4×10^{-11}	23
$[Dy(H_3NAP)_2Cl_2]Cl\cdot EtOH$	1200	22.9 K	2.9×10^{-6}	24
$[Dy(H_3NAP)_2(H_2O)Cl_2]Cl\cdot 2CH_3CN\cdot MeOH\cdot 0.5H_2O$	1200	153.9 K	2.5×10^{-8}	24
$(Et_3NH)[Dy((R,R)\text{-}3\text{-}NO_2salcy)_2]$	1500; 200	39.9 K; 18.2 K	3.62×10^{-6}; 2.92×10^{-5}	25
$[Dy(Bpen)(Cl)_3]$	800	22.4	3.7×10^{-6}	26
$[Dy(Bpen)Cl(OPhCl_2NO_2)_2]$	1000	85.8	4.7×10^{-7}	26
$[Dy(Bpen)\ (OPhCl_2NO_2)_3]$	800	34.2	2.4×10^{-6}	26
$[Dy(Bpen)(OPhNO_2)_3]$	800	26.8	1.1×10^{-6}	26
$[Dy(NO_3)_2L]NO_3$	1000	24.1 K	9.1×10^{-8}	27

$[Dy(AcO)_2L]CF_3SO_3$	1000	85.3 K	1.1×10^{-10}	27
$[Dy(acac)_2L]CF_3SO_3$	1000	140.2 K	3.3×10^{-9}	27
$[Dy(nma)(NO_3)_2(DMSO)]\cdot CH_3OH$	2000	67 K	1.7×10^{-7}	28
$[Dy(nma)_2]\cdot ClO_4\cdot 0.5CH_3OH$	2000	16 K; 47 K	1.0×10^{-5}; 4.6×10^{-6}	28

Notes:

L = (*S*, *S*)-2,2′-Bis(4-benzyl-2-oxazoline)], FTA = 2-furyltrifluoro-acetonate;

N_5 = 2,13-dimethyl-3,6,9,12,18-penta-aza-bicyclo-[12.3.1]octadeca-1(18),2,12,14,16-penta-ene, N_3O_2 = 2,2′-(ethylenedioxy)bis(ethylamine), db-N_3O_3 = 2-{2-[2-(2-aminophenoxy)ethoxy]ethoxy}aniline, db = dibenzo;

TTA = 2-thenoyltrifluoroacetone and HL = N-(methylene-8-hydroxyquinoline)-pyridylhydrazone;

$L^{CO}H$ = {*N*-[(2-MeO)C_6H_5]}N=C(Me)CH=C(Me)N(H){*N*′-[(2-MeO)C_6H_5]}, HN* = $HN(SiMe_3)_2$;

L_1 = 2,4-di-tert-butyl-6-((quinolin-8-ylimino)methyl)phenolate, L_2 = 2,4-di-tert-butyl-6-(((pyridin-2-ylmethyl)imino)methyl)phenolate;

NAS= 2-naphthalenesulfonate;

hniH = 2-(hydroxyl-3-methoxy-5-nitrophenyl)methylene(isonictino)hydrazine;

salanH = salicylideneaniline;

H_2TBPP = 5,10,15,20- tetrakis(4-tert-butylphenyl)porphyrin and H_2L = *N*,*N*′-bis(3-methoxysalicylidene) benzene-1,2-diamine;

H_2L = [2,6-diylbis(ethan-1-yl-1-ylidene)di(isonicotinohydrazide)];

H_2L^{OCH3} = 1,1′-(pyridine-2,6-diyl)bis(ethan-1-yl-1-ylidene))di-4-methoxybenzohydrazine;

H_2dapsc = 2,6-diacetylpyridine bis(semicarbazone);

H_2L = *N*,*N*′,*N*″-trimethyl-*N*,*N*′-bis(2-hydroxy-3-methoxy5-methylbenzyl) diethylene triamine;

H_2bpdc =2,2′-bipyridine-6,6′-dicarboxylic acid;

12-crown-4 = 1,4,7,10-tetraoxacyclododecane;

Hhmb = (*N*′-(2-hydroxy-3-methoxybenzylidene)-Benzohydrazide;

H_4L = 2,2′-{[(2-aminoethyl)imino]bis[2,1-ethanediyl-nitriloethylidyne]}bis-2- hydroxy-benzoic acid;

H_3NAP = 1,3-bis(2-hydroxynaphthalenemethyleneamino)-propan-2-ol;

3-NO_2salcyH_2 = *N*, *N*′-(1,2-cyclohexanediylethylene)bis(3-nitrosalicylideneiminato);

Bpen = *N*,*N*′-bis(2-methylenepyridinyl)ethylenediamine, $HOPhCl_2NO_2$ = 2,6-dichloro-4-nitrophenol, $HOPhNO_2$ = *p*-nitrophenol;

L denotes Schiff-base N_5 ligand;

Hnma = *N*-(2-(8-hydroxylquinolinyl)methane)2-)4-imidazolyl)ethanamine))).

Table S2 The CShMs values calculated with the program SHAPE[29] for each geometry for complexes **1Dy**-**4Dy**.

Complex	**1Dy**	**2Dy**	**3Dy**	**4Dy**
JCSAPR	4.223	4.160	3.181	3.357
CSAPR	3.400	3.167	**2.410**	2.593
JTCTPR	**3.197**	4.600	4.030	3.587
TCTPR	3.722	3.550	3.354	3.664
MFF	3.311	**3.003**	2.428	**2.371**

Notes: JCSAPR, C_{4v} Capped square antiprism; CSAPR, C_{4v} Spherical capped square antiprism; JTCTPR, D_{3h} Tricapped trigonal prism; TCTPR, Spherical tricapped trigonal prism; MFF, C_s, muffin.

Table S3 Extracted parameters from the Cole-Cole plots with the generalized Debye functions for **1Dy** under a 1 kOe dc field.

T (K)	χ_s (cm^3mol^{-1})	χ_T (cm^3mol^{-1})	α	τ (s)
7	7.69036140E-02	1.85324646E+00	1.03234957E-01	1.14729609E-03
7.5	8.02958068E-02	1.66272508E+00	7.41706886E-02	6.54979645E-04
8	7.73758049E-02	1.54292248E+00	6.74838991E-02	4.12291974E-04
8.5	7.68584337E-02	1.43973322E+00	5.81056316E-02	2.66903101E-04
9	7.33278801E-02	1.36682095E+00	5.90838824E-02	1.79460645E-04
9.5	7.39398252E-02	1.28230369E+00	4.81913107E-02	1.20711875E-04
10	7.12054579E-02	1.22297789E+00	4.80937124E-02	8.36497079E-05
10.5	7.02363945E-02	1.15886544E+00	4.07501222E-02	5.80690002E-05
11	6.90869709E-02	1.10735331E+00	3.71498285E-02	4.09055413E-05
11.5	6.62500386E-02	1.05966072E+00	3.46367117E-02	2.90423578E-05
12	6.91056249E-02	1.01567200E+00	2.83085520E-02	2.08955287E-05

Table S4 Extracted parameters from the Cole-Cole plots with the generalized Debye functions for **2Dy** under a 2 kOe dc field.

T (K)	χ_s (cm^3mol^{-1})	χ_T (cm^3mol^{-1})	α	τ (s)
6	7.74059542E-02	1.98488227E+00	8.99841565E-02	8.38579805E-04
6.5	8.21250973E-02	1.80980803E+00	7.29668667E-02	4.25052555E-04
7	8.30663015E-02	1.67768929E+00	6.76746494E-02	2.21104617E-04
7.5	8.38838333E-02	1.55867051E+00	6.05828098E-02	1.14933264E-04
8	7.76210819E-02	1.46632060E+00	6.24540385E-02	6.06892503E-05
8.5	7.75607183E-02	1.37952543E+00	5.49062960E-02	3.26590575E-05
9	7.14142947E-02	1.30777241E+00	5.31522565E-02	1.80712233E-05

Table S5 Extracted parameters from the Cole-Cole plots with the generalized Debye functions for **3Dy** under a 2 kOe dc field.

T (K)	χ_s (cm^3mol^{-1})	χ_T (cm^3mol^{-1})	α	τ (s)
3.25	4.23439513E-02	2.36365417E+00	1.46257978E-01	1.29889887E-03
3.50	4.16998911E-02	2.26723546E+00	1.37020696E-01	8.23058732E-04
3.75	4.08843270E-02	2.15954882E+00	1.28234536E-01	5.11009955E-04
4.00	4.11086275E-02	2.05003493E+00	1.18785727E-01	3.13903767E-04
4.25	3.75788790E-02	1.95729244E+00	1.15706320E-01	1.92780231E-04
4.50	3.38518087E-02	1.87122317E+00	1.14060698E-01	1.17478248E-04
4.75	2.88857513E-02	1.77953631E+00	1.10045317E-01	7.04941507E-05
5.00	1.86118904E-02	1.70290045E+00	1.10189064E-01	4.24136098E-05
5.25	3.58103129E-03	1.63078495E+00	1.10644746E-01	2.54664713E-05

Table S6 Extracted parameters from the Cole-Cole plots with the generalized Debye functions for **4Dy** under a 2 kOe dc field.

T (K)	χ_s (cm^3mol^{-1})	χ_T (cm^3mol^{-1})	α	τ (s)
3.25	5.98536969E-02	2.87421802E+00	7.96263036E-02	1.37829627E-03
3.50	5.80285274E-02	2.82395895E+00	8.31917713E-02	9.77600959E-04
3.75	5.67402224E-02	2.74610938E+00	8.84741512E-02	6.63068992E-04
4.00	5.11118862E-02	2.62241058E+00	9.42915381E-02	4.37701993E-04
4.25	3.90471076E-02	2.51909432E+00	1.10423142E-01	2.86921325E-04
4.50	1.98567052E-02	2.45405646E+00	1.34064479E-01	1.89540396E-04
4.75	2.43788616E-12	2.34981688E+00	1.49713336E-01	1.20944078E-04
5.00	7.52863604E-24	2.24706633E+00	1.58019190E-01	7.75481442E-05
5.25	3.03620811E-26	2.14851318E+00	1.66184990E-01	4.95630746E-05
5.50	4.64481301E-27	2.05692364E+00	1.74026000E-01	3.18672195E-05
5.75	8.84819547E-13	1.98444876E+00	1.84457363E-01	2.07849203E-05

Table S7 Calculated energy levels (cm^{-1}), $\boldsymbol{g}$ (g_x, g_y, g_z) tensors and predominant m_J values of the lowest eight Kramers doublets (KDs) of complexes **1Dy**−**4Dy** using CASSCF/RASSI-SO with MOLCAS 8.4[1-2].

KDs	**1Dy**			**2Dy**			**3Dy**			**4Dy**		
	E	**g**	m_J	*E*	**g**	m_J	*E*	**g**	m_J	*E*	**g**	m_J
		0.0755			0.119			0.105			1.121	
1	0.0	0.0955	±15/2	0.0	0.190	±15/2	0.0	0.228	±15/2	0.0	3.102	±15/2
		19.678			**19.720**			**19.665**			**16.154**	
		1.022			1.215			0.773			0.672	
2	93.8	1.488	±13/2	70.5	1.878	±13/2	46.1	2.425	±9/2	25.9	2.659	±1/2
		15.699			15.821			14.679			14.450	
		0.481			2.608			0.446			2.182	
3	176.3	1.208	±1/2	144.7	3.954	±1/2	67.6	3.159	±11/2	63.7	3.495	±7/2
		11.133			12.785			11.884			14.263	
		0.293			8.995			3.354			1.375	
4	218.6	4.136	±5/2	213.8	5.424	±11/2	139.5	5.057	±13/2	86.2	4.915	±3/2
		11.337			0.826			9.768			12.101	
		1.742			0.837			9.892			0.784	
5	268.8	4.023	±11/2	248.4	2.612	±5/2	180.2	5.355	±1/2	133.7	4.229	±5/2
		9.729			15.007			0.601			13.077	
		2.294			2.530			1.826			1.068	
6	323.1	3.097	±9/2	290.3	3.223	±9/2	214.7	1.958	±7/2	156.6	3.250	±9/2
		14.814			14.087			13.665			11.264	
		3.243			1.780			1.330			3.351	
7	351.8	5.539	±7/2	341.4	4.196	±3/2	280.1	2.868	±5/2	196.2	5.561	±11/2
		11.935			9.430			13.698			11.554	
		0.1958			1.739			0.720			0.223	
8	462.1	0.2560	±3/2	380.5	5.709	±7/2	341.5	0.825	±3/2	264.4	0.596	±13/2
		18.953			13.920			17.273			**18.384**	

Table S8 Wave functions with definite projection of the total moment | m_J > and QTM components for the lowest two KDs of complexes **1Dy**−**4Dy**.

	E	wave functions	QTM components
1Dy	0.0	98.1%|±15/2>	0.029
	93.8	86.8%|±13/2>+4.6%|±3/2>+2.8%|±1/2>+2.0%|±11/2>+1.5%|±5/2>	0.42
2Dy	0.0	98.5%|±15/2>	0.051
	70.5	90.1%|±13/2>+3.3%|±1/2>	0.52
3Dy	0.0	98.4%|±15/2>	0.056
	46.1	25.8%|±13/2>+16.1%|±3/2>+15.6%|±1/2>+12.7%|±5/2>+10%|±7/2>+ 9.7%|±11/2>+9.6%|±9/2>	2.4
4Dy	0.0	73.5%|±15/2>+8.4%|±9/2>+7.4%|±7/2>+6%|±5/2>	0.7
	25.9	29.7%|±5/2>+22.1%|±7/2>+16.4%|±3/2>+13.4%|±15/2>+6.9%|±9/2>	2.0

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