Supplementary information

The effect of co-ligands on the performance of single-molecule magnet behaviours in a family of linear trinuclear Zn-Dy-Zn complexes with a compartmental Schiff base

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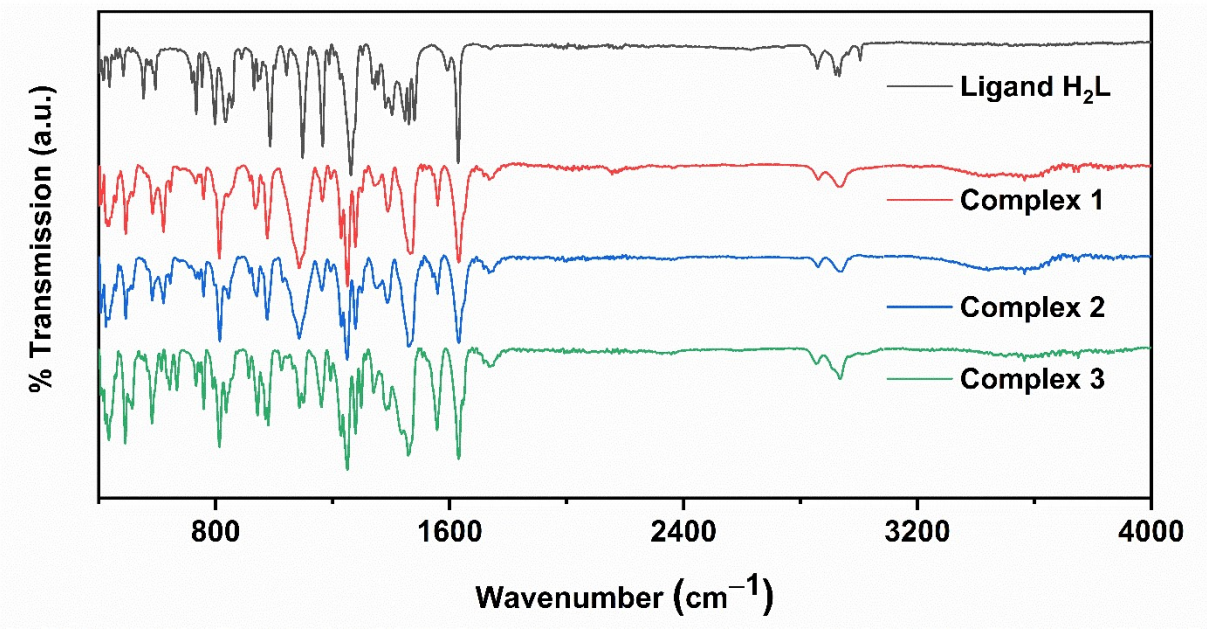

Fig. S1. IR spectra of ligand H_2L and complexes **1-3**.

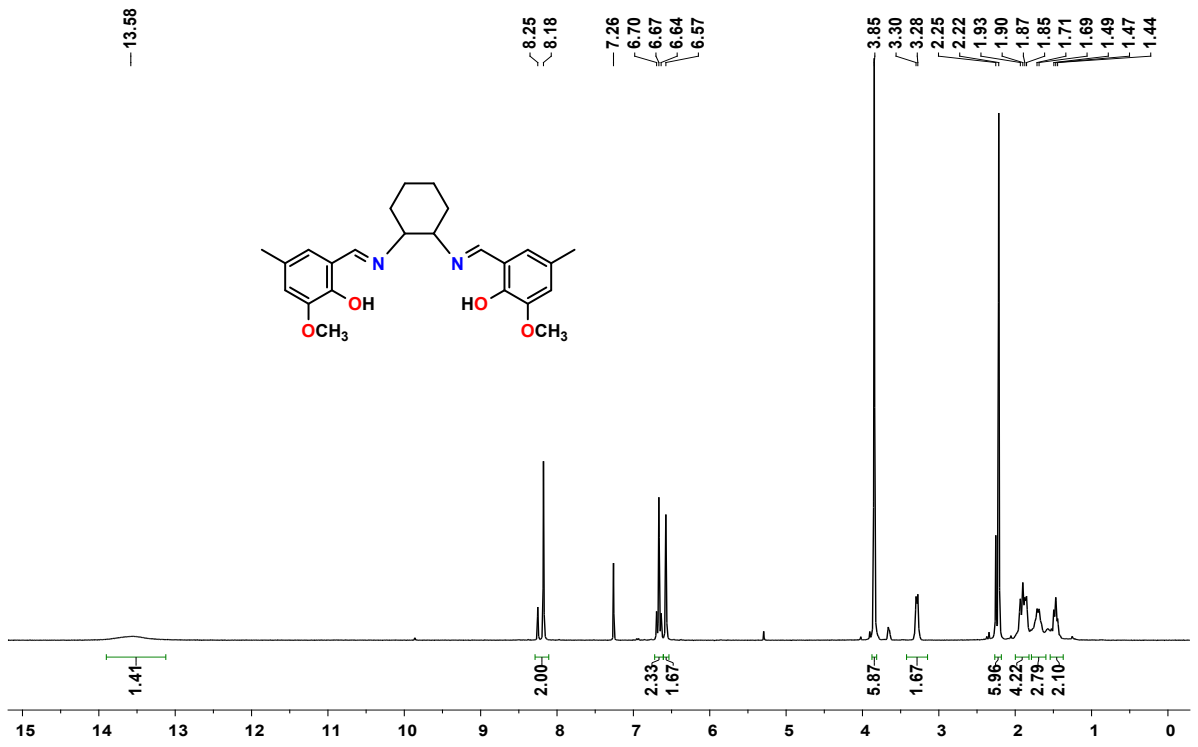

Fig. S2. ^{1}H-NMR of *N,N′*-bis(3-methoxy-5-methylsalicylidene)-1,2-diaminocyclohexane (H_2L) in $CDCl_3$ at r.t.

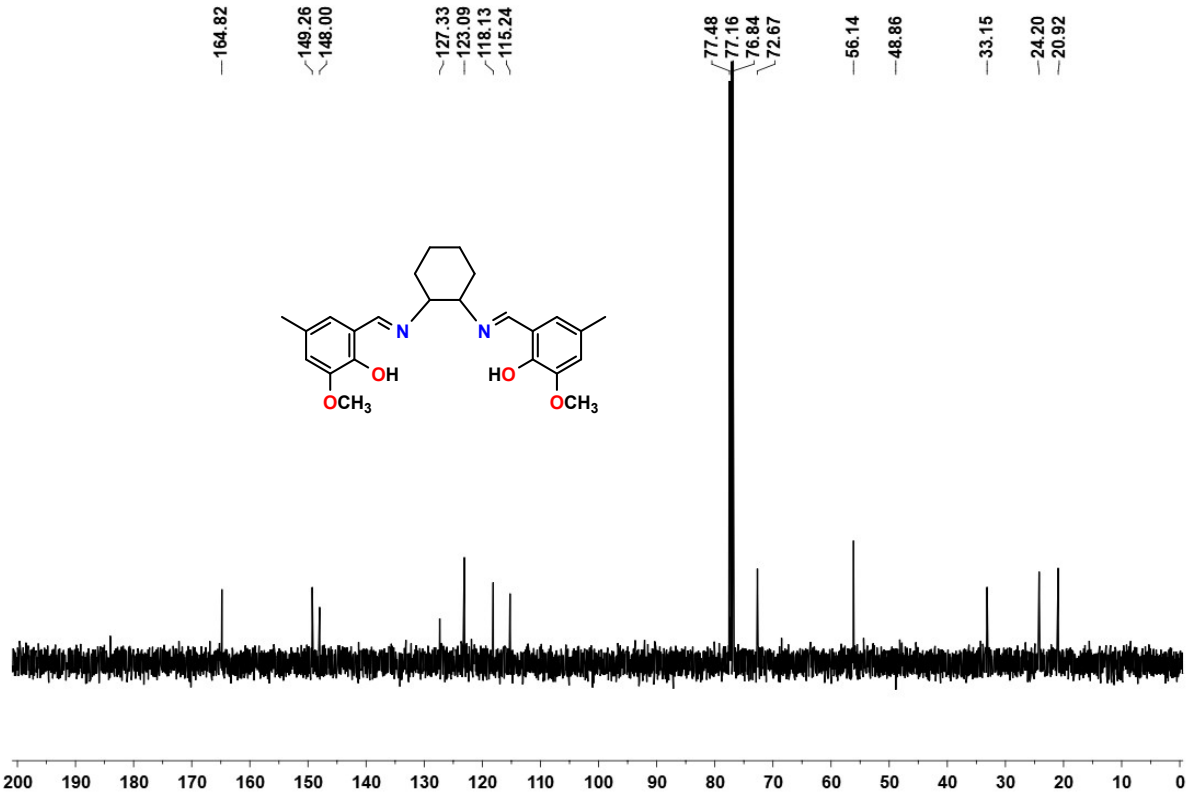

Fig. S3. ^{13}C-NMR of N,N'-bis(3-methoxy-5-methylsalicylidene)-1,2-diaminocyclohexane (H_2L) in $CDCl_3$ at r.t.

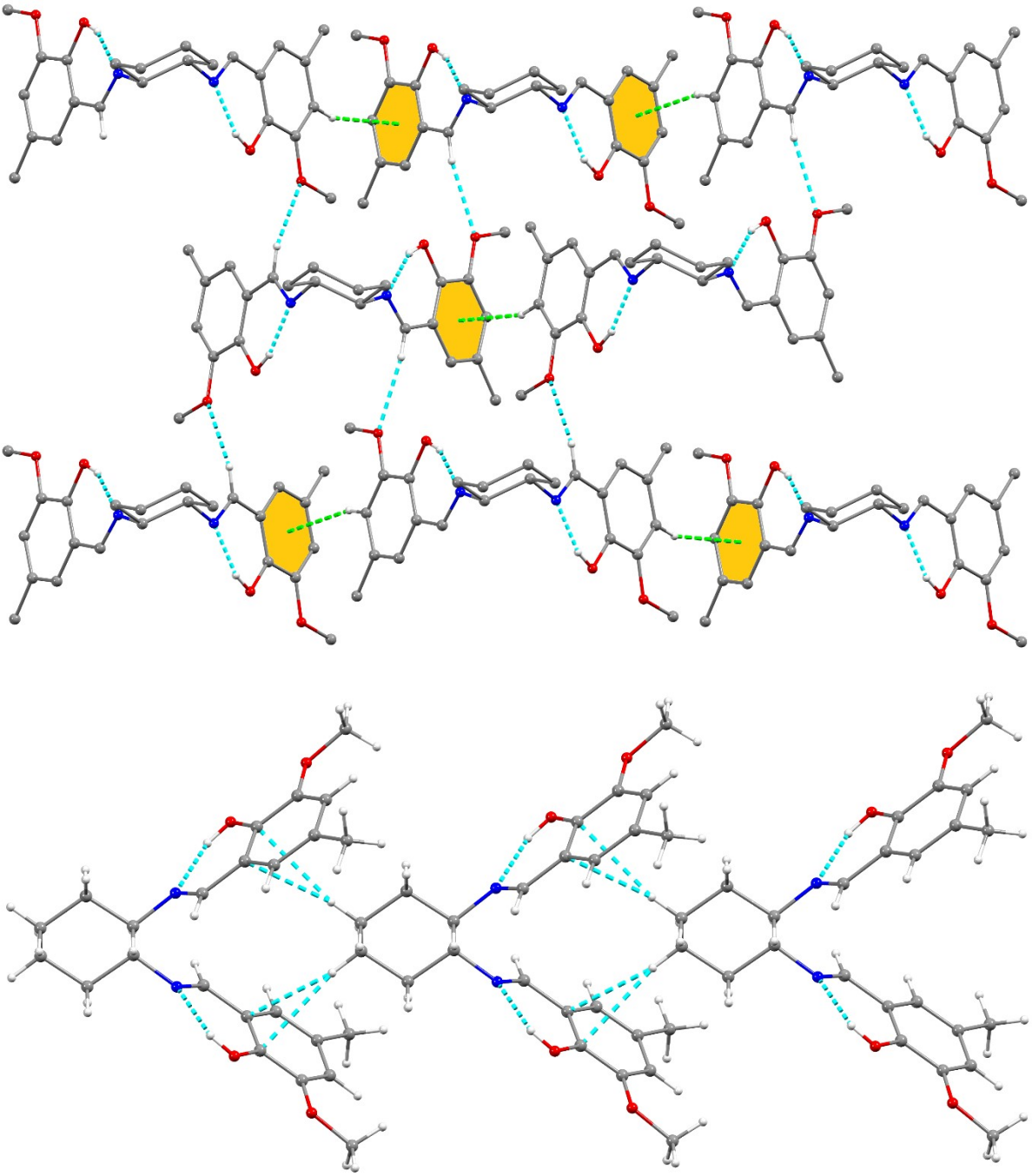

Fig. S4. Non-covalent interactions in the Schiff base ligand H_2L.

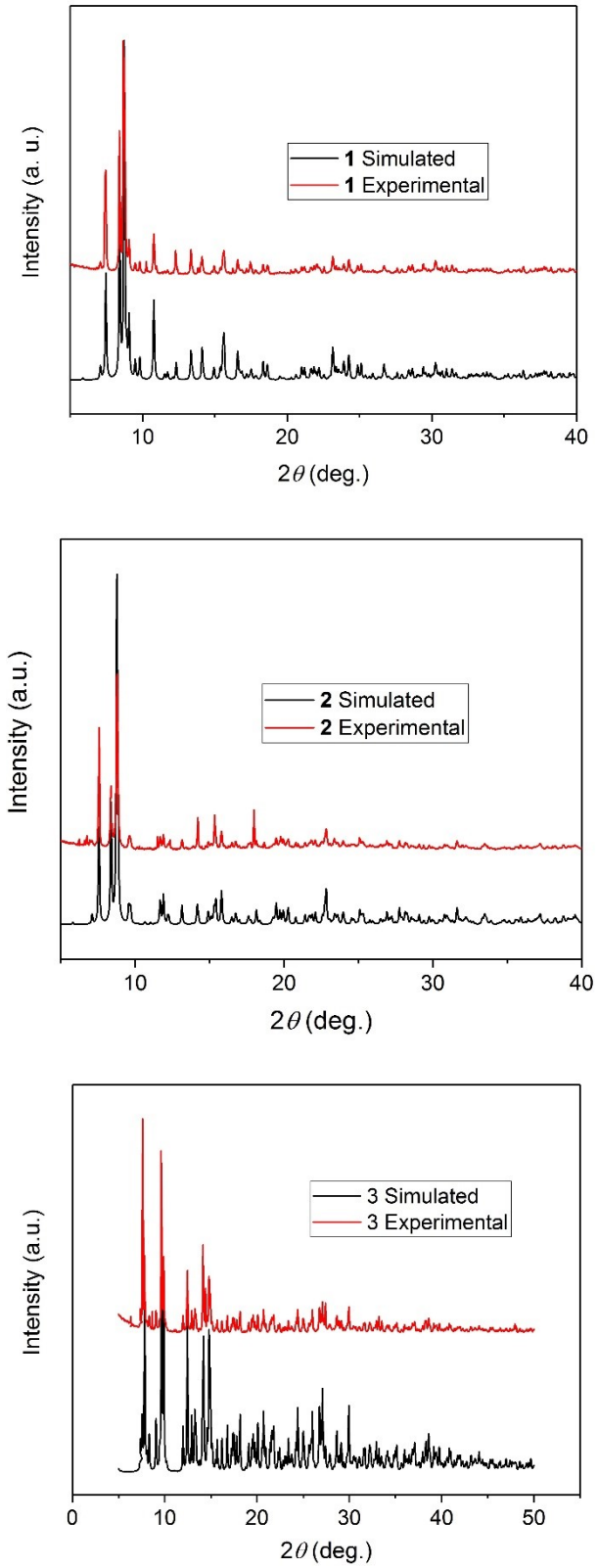

Fig. S5. Simulated and experimental PXRD data for **1-3**.

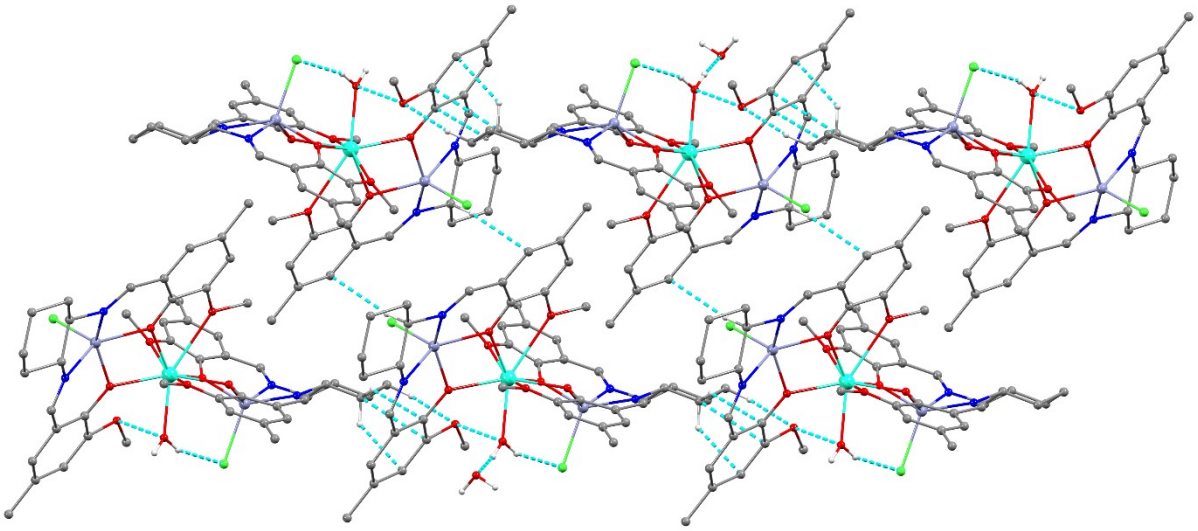

Fig. S6. Crystal packing diagram for complex **1**.

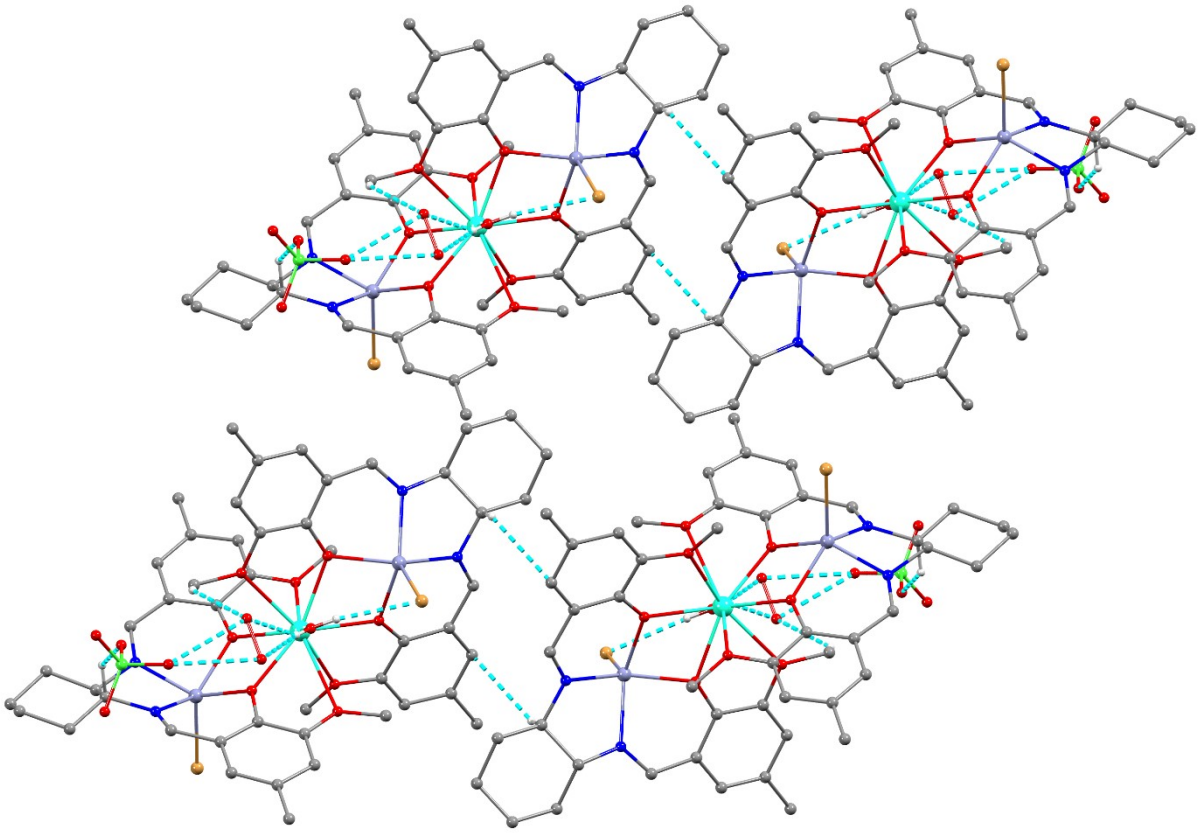

Fig. S7. Crystal packing diagram for complex **2**.

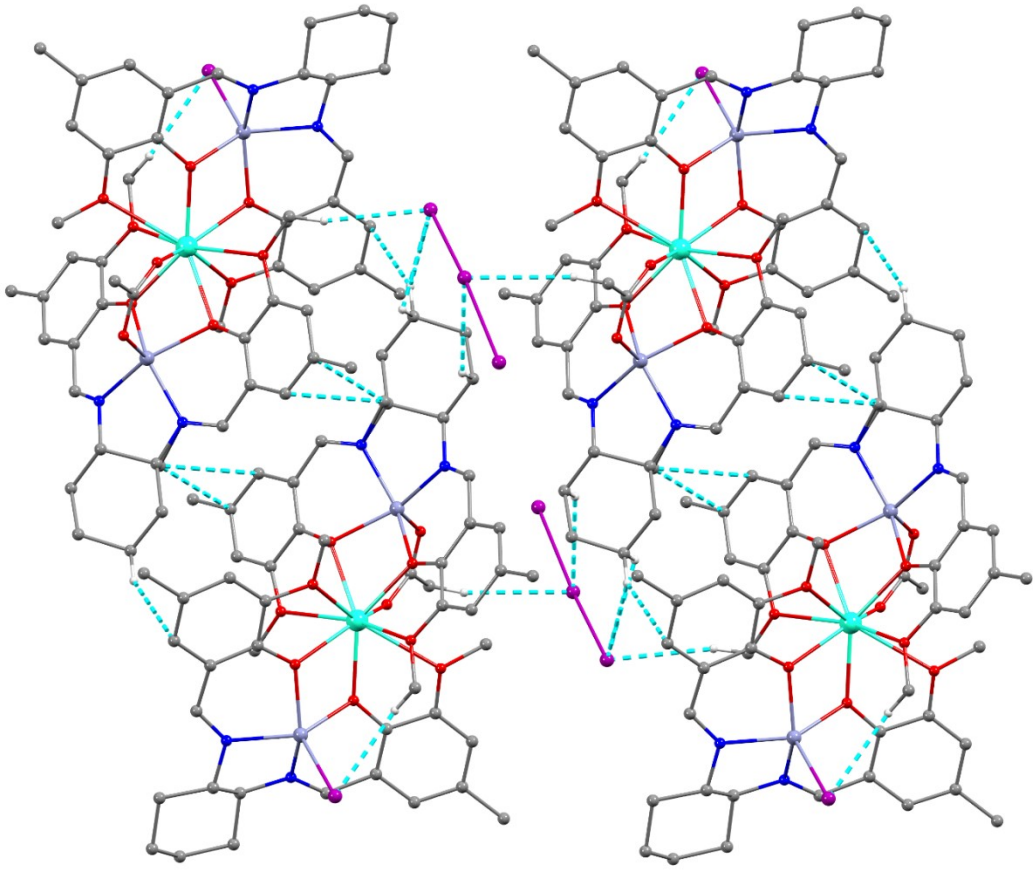

Fig. S8. Crystal packing diagram for complex **3**.

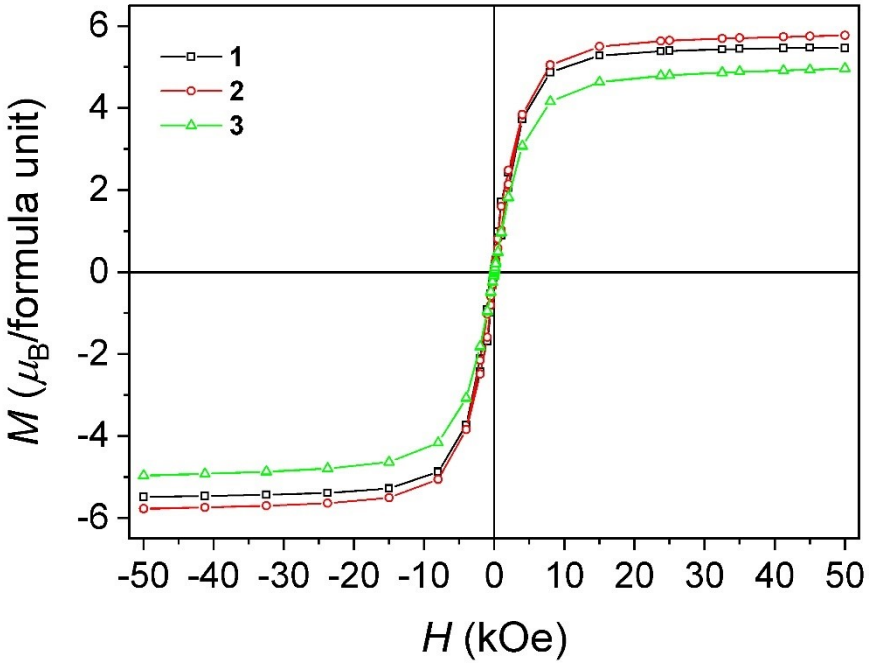

Fig. S9. Isothermal magnetization plots at 2 K for **1-3**.

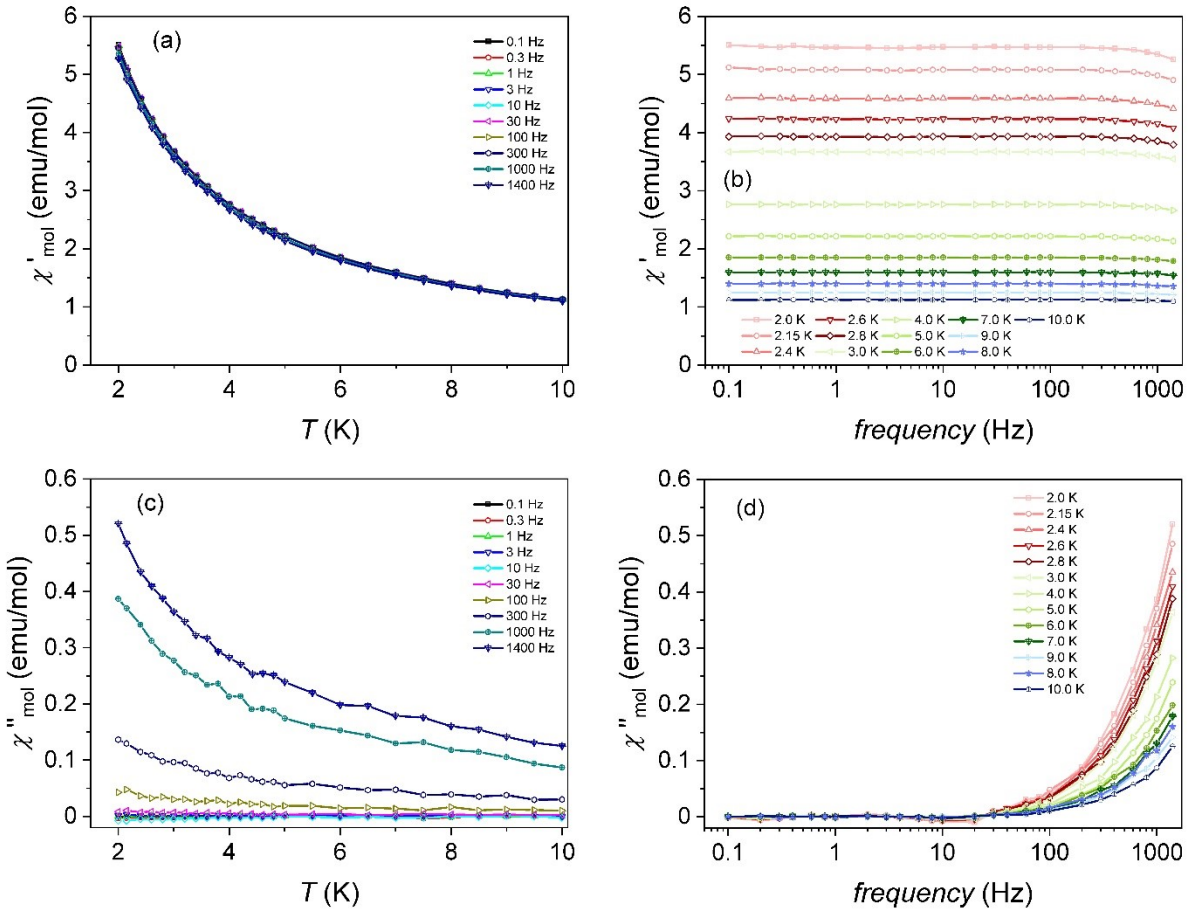

Fig. S10. AC data for complex **3** at zero dc field.

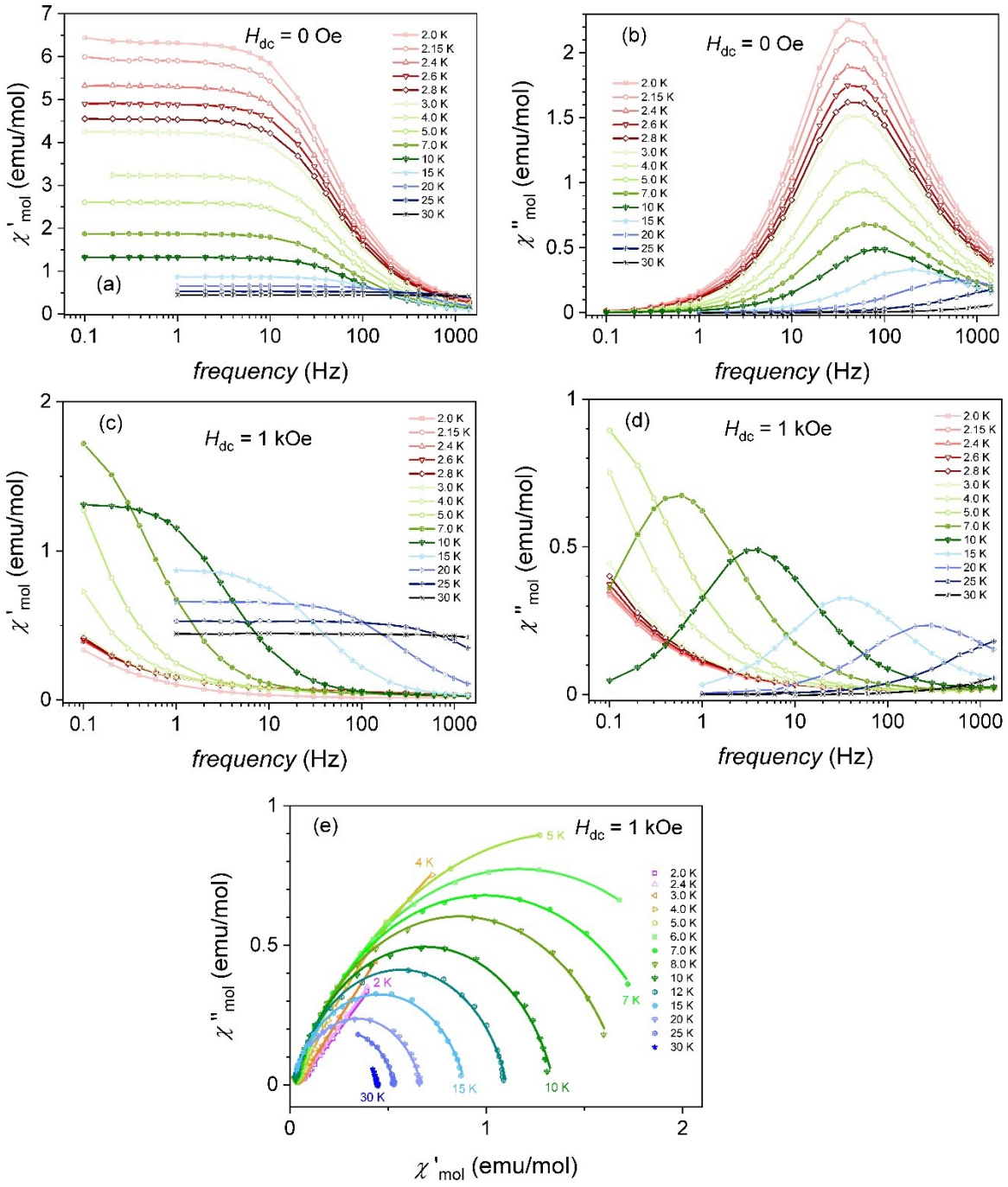

Fig. S11. In-phase (a) and out-of-phase (b) ac susceptibility for **1** as a function of ac frequencies in zero dc field and the corresponding plots in a 1000 Oe dc field (c and d) with only selected sets of temperatures for clarity. The Cole-Cole plots at 1000 Oe dc field (e).

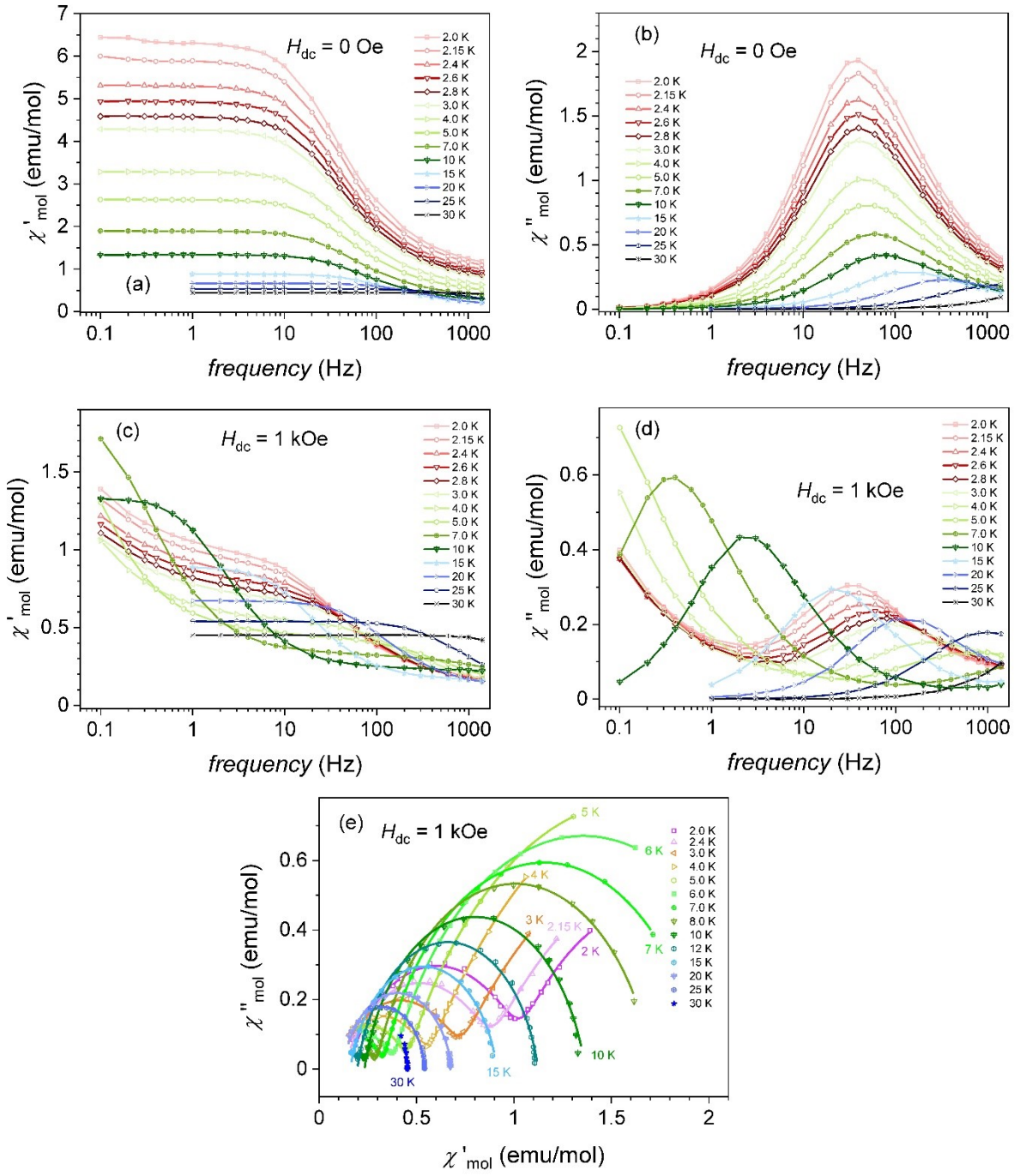

Fig. S12. In-phase (a) and out-of-phase (b) ac susceptibility for **2** as a function of ac frequencies in zero dc field and the corresponding plots in a 1000 Oe dc field (c and d) with only selected sets of temperatures for clarity. The Cole-Cole plots at 1000 Oe dc field (e).

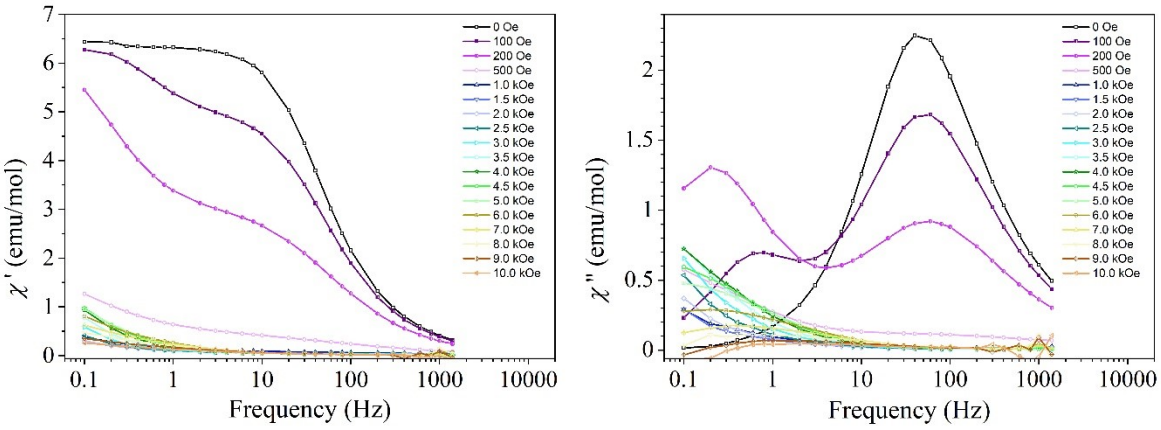

Fig. S13. The plots of χ″ as a function of ac frequency for different applied magnetic fields and at 2 K for **1**.

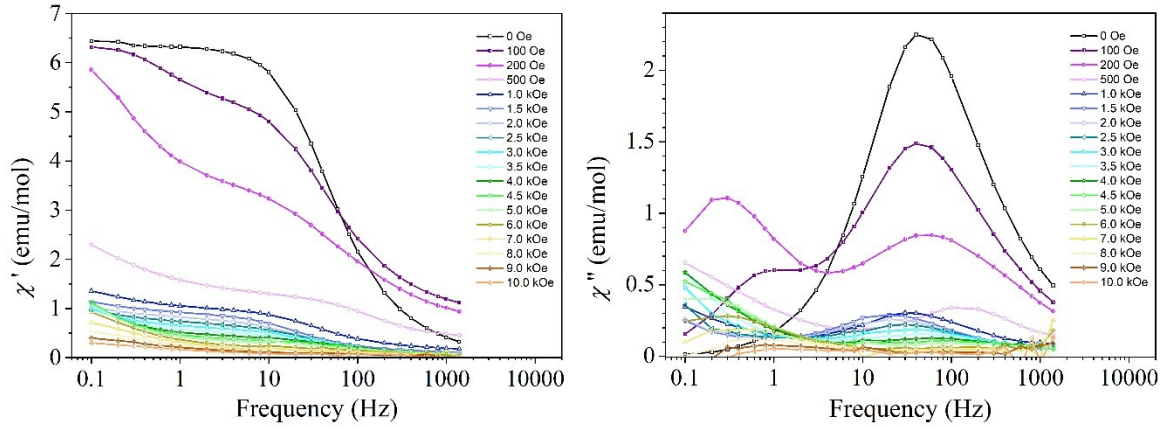

Fig. S14. The plots of χ″ as a function of ac frequency for different applied magnetic fields and at 2 K for **2**.

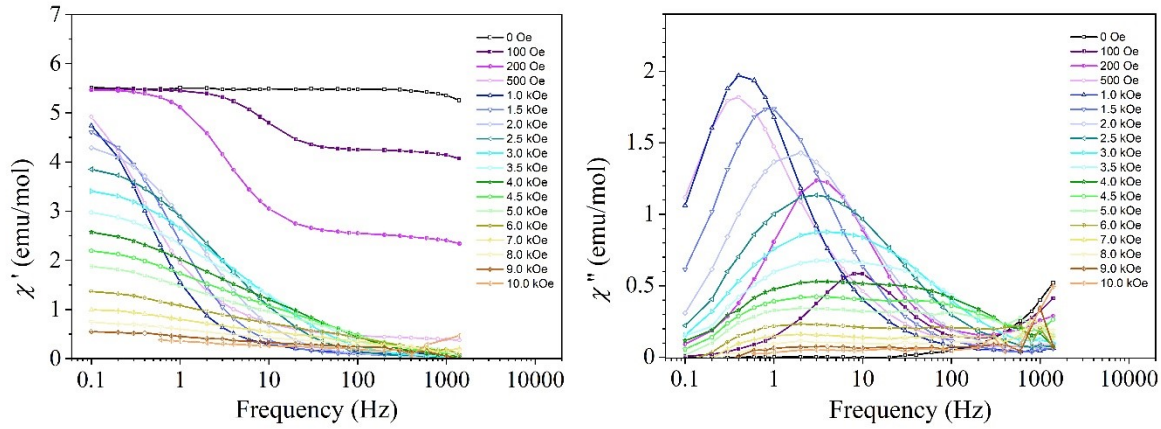

Fig. S15. The plots of χ″ as a function of ac frequency for different applied magnetic fields and at 2 K for **3**.

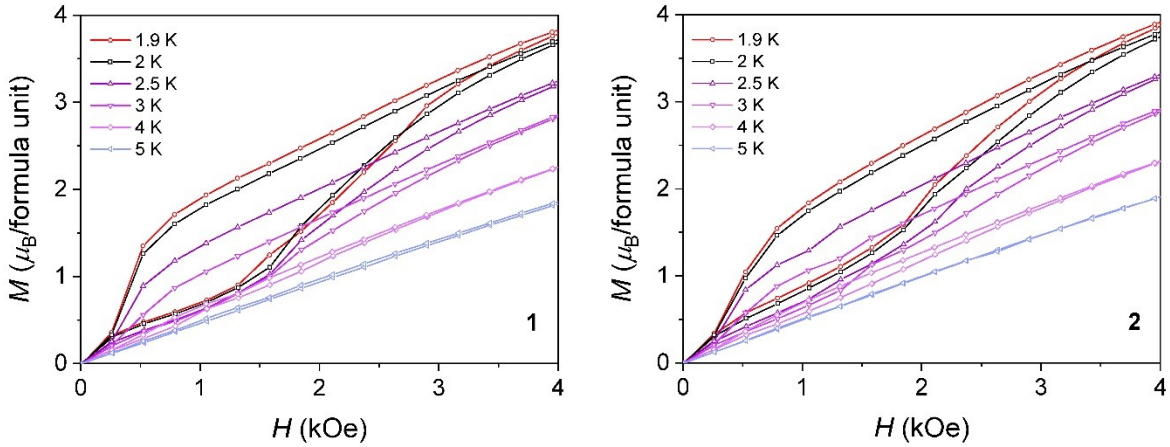

Fig. S16. Field dependence of magnetization of **1** (left) and **2** (right) at different temperatures. The magnetization plots in the positive directions have only been shown.

Table S1. Crystallographic data and structure refinement parameters of **1−4.**

	H_2L	**1**	**2**	**3**
Empirical formula	$C_{24}H_{30}N_2O_4$	$C_{48}H_{60.05}Cl_3DyN_4O_{17}Zn_2$	$C_{48}H_{62}Br_2ClDyN_4O_{17}Zn_2$	$C_{50}H_{67}DyI_4N_4O_{14}Zn_2$
Formula weight	410.50	1370.68	1455.52	1748.91
Temperature/K	150.00	150.00	150.00	150.00
Crystal system	orthorhombic	monoclinic	monoclinic	triclinic
Space group	*Fdd*2	$P2_1/c$	$P2_1/c$	$P\bar{1}$
a/Å	20.8442(10)	12.5292(15)	12.5327(7)	12.5913(11)
b/Å	25.538(2)	19.500(2)	19.9571(11)	13.6488(12)
c/Å	8.7128(5)	23.808(3)	23.5431(12)	19.5604(17)
α/°	90	90	90	103.066(3)
β/°	90	95.720(4)	97.405(2)	94.469(3)
γ/°	90	90	90	114.008(3)
Volume/Å^3	4637.9(5)	5787.8(12)	5839.4(5)	2936.2(5)
Z	8	4	4	2
ρ_{calc} g/cm^3	1.176	1.573	1.656	1.978
μ/mm^{-1}	0.080	2.307	3.563	4.236
F(000)	1760.0	2780.0	2908.0	1690.0
2Θ range for data collection/°	5.046 to 54.242	5.304 to 60.452	4.912 to 61.128	4.532 to 58.506
Reflections collected	25447	234637	295248	189984
Independent reflections	2548 [R_{int} = 0.0215, R_{sigma} = 0.0097]	12768 [R_{int} = 0.0403, R_{sigma} = 0.0129]	17826 [R_{int} = 0.0382, R_{sigma} = 0.0155]	15903 [R_{int} = 0.0345, R_{sigma} = 0.0159]
Data/restraints/parameter	2548/1/146	12766/76/703	17826/123/741	15903/63/703
Goodness-of-fit on F^2	1.032	1.123	1.189	1.067
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0304, wR_2 = 0.0861	R_1 = 0.0513, wR_2 = 0.1187	R_1 = 0.0474, wR_2 = 0.1184	R_1 = 0.0441, wR_2 = 0.1152
Final R indexes [all data]	R_1 = 0.0312, wR_2 = 0.0870	R_1 = 0.0561, wR_2 = 0.1228	R_1 = 0.0581, wR_2 = 0.1275	R_1 = 0.0515, wR_2 = 0.1232
Largest diff. peak/hole / e Å^{-3}	0.23/-0.15	1.46/-1.58	1.38/-1.17	1.94/-1.96

Table S2. Selected bond parameters around the metal centres in **1−3**.

Bonds	**1**	**2**	**3**
Dy–O1 (phenoxo)	2.224(3)	2.321(3)	2.314(4)
Dy –O2 (methoxy)	2.491(3)	2.608(3)	2.645(4)
Dy –O3 (phenoxo)	2.407(3)	2.275(3)	2.291(4)
Dy –O4 (methoxy)	2.388(3)	2.772(3)	2.723(4)
Dy –O5(phenoxo)	2.421(4)	2.303(3)	2.289(4)
Dy –O6 (methoxy)	2.896(4)	2.538(3)	2.572(4)
Dy –O7 (phenoxo)	2.248(3)	2.307(3)	2.347(4)
Dy –O8 (methoxy)	2.816(4)	2.578(3)	2.600(4)
Dy –O9 (aqua)	2.375(4)	2.397(3)	–
Dy –O10 (acetate)	–	–	2.327(4)
Dy···Zn1	3.4302(7)	3.5549(5)	3.5516(11)
Dy···Zn2	3.5295(7)	3.4532(5)	3.302(12)

Table S3. Shape analysis of the structure **1-3.**

Label	**Shape**	**Symmetry**	**1**	**2**	**3**
EP-9	Enneagon	D_{9h}	32.617	36.181	35.493
OPY-9	Octagonal pyramid	C_{8V}	19.977	20.848	22.164
HBPY-9	Heptagonal bipyramid	D_{7h}	16.612	17.104	15.058
JTC-9	Johnson triangular cupola J3	C_{3v}	16.094	14.079	13.136
JCCU-9	Capped cube J8	C_{4V}	8.098	7.515	7.275
CCU-9	Spherical-relaxed capped cube	C_{4V}	7.827	7.000	6.866
JCSAPR-9	Capped square antiprism J10	C_{4V}	3.935	3.346	3.081
CSAPR-9	Spherical capped square antiprism	C_{4V}	3.743	2.763	2.879
JTCTPR-9	Tricapped trigonal prism J51	D_{3h}	5.307	3.833	4.358
TCTPR-9	Spherical tricapped trigonal prism	D_{3h}	**2.758**	**2.167**	2.792
JTDIC-9	Tridiminished icosahedron J63	C_{3V}	9.735	9.925	9.417
HH-9	Hula-hoop	C_{2V}	11.180	10.270	10.736
MFF-9	Muffin	C_S	3.580	2.822	**2.194**

Table S4. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **1** by the single-component generalized Debye model at zero and 1000 Oe dc fields.

T (K)	χ_S (emu/mol)	$\Delta\chi$ (emu/mol)	τ (s)	α	χ_S (emu/mol)	$\Delta\chi$ (emu/mol)	τ (s)	α
	H_{dc} = 0 Oe				H_{dc} = 1 kOe			
2	0.26279	6.15952	0.00302	0.185	0.04401	33502.77	1.75E+10	0.51743
2.15	0.24366	5.74847	0.00299	0.18645	0.04218	38604.74	1.73E+10	0.5114
2.4	0.22357	5.15458	0.00292	0.1832	0.04003	40280.48	1.30E+10	0.50468
2.6	0.2105	4.74854	0.00287	0.18165	0.0393	273712.2	3.18E+11	0.49353
2.8	0.19633	4.40567	0.00282	0.18201	0.0382	45177.1	4.97E+09	0.48205
3	0.18152	4.11301	0.00278	0.18255	0.03804	15123.69	2.81E+08	0.46537
3.2	0.17188	3.86762	0.00274	0.18306	0.03694	978.2859	1025221	0.45238
3.4	0.16389	3.66707	0.0027	0.18251	0.03762	16.53743	349.5559	0.42414
3.6	0.15625	3.49284	0.00265	0.18309	0.03885	8.37992	68.43573	0.39505
3.8	0.1524	3.29965	0.0026	0.18065	0.03966	5.6118	24.03877	0.36527
4	0.14274	3.13232	0.00256	0.18175	0.03974	4.33411	11.45507	0.33752
4.2	0.13809	2.98067	0.00253	0.18107	0.03998	3.77909	7.1154	0.31715
4.4	0.13043	2.85412	0.0025	0.18272	0.03929	3.37786	4.74812	0.30001
4.6	0.13151	2.72744	0.00245	0.1777	0.03822	3.13034	3.43647	0.28711
4.8	0.12638	2.61593	0.00242	0.17812	0.03712	2.93857	2.57921	0.27674
5	0.12093	2.51317	0.00238	0.17774	0.03679	2.78259	1.98199	0.26655
5.5	0.11252	2.28407	0.00229	0.17723	0.03468	2.49775	1.12016	0.25083
6	0.10461	2.09275	0.0022	0.17547	0.03278	2.26904	0.67444	0.2379
6.5	0.10056	1.93374	0.00213	0.17374	0.03143	2.08343	0.43218	0.22681
7	0.09287	1.79918	0.00205	0.17253	0.03017	1.92195	0.28584	0.21674
7.5	0.08866	1.67919	0.00198	0.1713	0.02929	1.78879	0.19568	0.20902
8	0.08527	1.57433	0.0019	0.16831	0.02854	1.66816	0.13692	0.20229
8.5	0.08006	1.4849	0.00182	0.16824	0.02824	1.56563	0.09843	0.19562
9	0.07768	1.40368	0.00175	0.16508	0.02812	1.47444	0.07225	0.19024
9.5	0.07451	1.3302	0.00167	0.16213	0.02744	1.39386	0.05396	0.18538
10	0.0722	1.26259	0.00159	0.15831	0.0268	1.31828	0.04059	0.18012
10.5	0.0505	1.18588	0.00144	0.15531	0.02831	1.24488	0.03132	0.17156
11	0.06705	1.1326	0.00137	0.15346	0.02612	1.188	0.02405	0.17771
11.5	0.06442	1.08272	0.0013	0.14886	0.02538	1.13623	0.01905	0.17588
12	0.06131	1.03075	0.00121	0.14607	0.02572	1.07727	0.01413	0.16815
12.5	0.05857	0.99168	0.00114	0.14279	0.02373	1.03657	0.01156	0.17439
13	0.05578	0.95561	0.00107	0.14134	0.0249	0.99537	0.00931	0.16783
13.5	0.05282	0.92103	9.99E-04	0.13838	0.02271	0.9623	0.00766	0.17209
14	0.05057	0.88902	9.26E-04	0.13638	0.02309	0.92509	0.00616	0.16848
14.5	0.04883	0.85873	8.57E-04	0.13402	0.02014	0.89498	0.00503	0.17604
15	0.04229	0.83923	7.88E-04	0.13934	0.01573	0.87621	0.00417	0.18917
15.5	0.0407	0.81263	7.21E-04	0.13766	0.01772	0.84922	0.0034	0.18301
16	0.03802	0.78847	6.56E-04	0.13716	0.01975	0.82017	0.00277	0.17813

16.5	0.03732	0.76421	5.95E-04	0.13514	0.01771	0.7946	0.00227	0.18425
17	0.03532	0.74285	5.36E-04	0.13497	0.01729	0.77069	0.00187	0.18997
17.5	0.03407	0.72184	4.82E-04	0.13532	0.01789	0.74962	0.00152	0.18909
18	0.03211	0.70316	4.31E-04	0.13564	0.01787	0.72796	0.00125	0.19177
18.5	0.03194	0.68274	3.82E-04	0.13702	0.01917	0.70353	0.00101	0.19042
19	0.02962	0.66671	3.38E-04	0.13731	0.01828	0.68496	8.26E-04	0.19517
19.5	0.03054	0.64745	2.99E-04	0.13825	0.01933	0.66668	6.77E-04	0.19764
20	0.0328	0.62834	2.64E-04	0.13757	0.02101	0.64677	5.52E-04	0.19461
20.5	0.02986	0.61524	2.30E-04	0.14189	0.02202	0.62783	4.50E-04	0.19585
21	0.02981	0.59965	2.01E-04	0.14224	0.02547	0.61003	3.70E-04	0.19702
21.5	0.03908	0.57546	1.79E-04	0.13737	0.02669	0.59247	3.03E-04	0.19484
22	0.03772	0.56289	1.54E-04	0.1419	0.0269	0.57893	2.48E-04	0.19529
22.5	0.03416	0.55337	1.33E-04	0.14354	0.0379	0.55268	2.09E-04	0.185
23	0.03494	0.53956	1.15E-04	0.1435	0.04029	0.53652	1.71E-04	0.1802
23.5	0.04168	0.52038	1.02E-04	0.13802	0.04183	0.52427	1.42E-04	0.17986
24	0.04308	0.50784	8.78E-05	0.1383	0.04243	0.51222	1.18E-04	0.17893
24.5	0.04339	0.49637	7.48E-05	0.14078	0.0436	0.49885	9.56E-05	0.17745
25	0.04316	0.4858	6.46E-05	0.13548	0.03685	0.49393	7.74E-05	0.17059
25.5	0.04857	0.47023	5.56E-05	0.13645	0.04914	0.47045	6.60E-05	0.15795
26	0.02953	0.47917	4.47E-05	0.14116	0.05549	0.45503	5.62E-05	0.15558
26.5	0.0461	0.45352	3.97E-05	0.14014	0.03793	0.46286	4.45E-05	0.15468
27	0.04024	0.45027	3.28E-05	0.14149	0.01929	0.47327	3.39E-05	0.16605
27.5	0.0306	0.45121	2.69E-05	0.14862	0.04624	0.4376	3.08E-05	0.15701
28	0.05536	0.41833	2.56E-05	0.12871	0	0.4753	2.18E-05	0.16909
28.5	0	0.46567	1.81E-05	0.14626	0.04233	0.42429	2.12E-05	0.1518
29	0	0.45843	1.52E-05	0.15063	0.02039	0.43856	1.67E-05	0.15791
29.5	0.06771	0.38364	1.57E-05	0.14903	0.05736	0.39312	1.61E-05	0.13653
30	0.10219	0.34147	1.72E-05	0.10766	0.05134	0.39334	1.33E-05	0.15385

Table S5. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **2** by the single-component generalized Debye model at zero and 1000 Oe dc fields**.**

T (K)	χ_S (emu/mol)	$\Delta\chi$ (emu/mol)	τ (s)	α	χ_S (emu/mol)	$\Delta\chi$ (emu/mol)	τ (s)	α
	H_{dc} = 0 Oe				H_{dc} = 1 kOe (LF)			
2	1.12328	5.29912	0.0035	0.19473	0.15039	1.41777	4.31932	0.26265
2.15	1.05742	4.91941	0.00345	0.18913	0.14331	1.51776	5.05189	0.29327
2.4	0.96128	4.41359	0.00338	0.18734	0.12732	1.99943	9.84324	0.3474
2.6	0.89186	4.10256	0.00331	0.18629	0.1174	1.90336	8.67553	0.34025
2.8	0.83387	3.80594	0.00326	0.1858	0.10723	2.28281	12.78964	0.36759
3	0.77924	3.55184	0.00319	0.18559	0.09666	2.29161	12.03096	0.35977
3.2	0.73395	3.35185	0.00314	0.18667	0.09135	2.75531	16.27422	0.37453
3.4	0.69873	3.18958	0.00308	0.18638	0.08304	2.76181	14.05481	0.36481
3.6	0.67008	3.03425	0.00301	0.18413	0.07945	3.04227	14.49693	0.35989
3.8	0.64122	2.8666	0.00294	0.18238	0.07579	3.23927	14.33641	0.3621
4	0.60754	2.71549	0.00288	0.182	0.0747	3.05869	10.44943	0.34135
4.2	0.57669	2.58662	0.00282	0.1821	0.06934	2.90432	7.89861	0.32456
4.4	0.55392	2.46551	0.00278	0.18153	0.05753	2.79948	6.21026	0.31152
4.6	0.53083	2.35798	0.00273	0.1813	0.05494	2.69993	4.92106	0.30188
4.8	0.51015	2.26055	0.00268	0.18087	0.05754	2.56289	3.77423	0.28923
5	0.4905	2.17255	0.00263	0.18093	0.05524	2.42096	2.89749	0.27553
5.5	0.45074	1.97118	0.00252	0.17902	0.04474	2.17099	1.63785	0.25458
6	0.41654	1.80533	0.00242	0.17708	0.01843	1.9517	0.97512	0.23378
6.5	0.38549	1.673	0.00232	0.17752	0	1.78231	0.62001	0.21658
7	0.3607	1.55472	0.00224	0.17708	0	1.6479	0.41443	0.20509
7.5	0.33867	1.45149	0.00216	0.17445	0	1.52208	0.28292	0.19107
8	0.32118	1.35903	0.00208	0.17227	0	1.41821	0.19974	0.18001
8.5	0.30292	1.28153	0.002	0.17123	0.26798	1.35076	0.14295	0.18463
9	0.29018	1.20947	0.00194	0.16773	0.25583	1.26899	0.10569	0.17591
9.5	0.27364	1.14977	0.00185	0.16742	0.24563	1.19783	0.07957	0.16798
10	0.26163	1.08863	0.00177	0.16403	0.23266	1.13297	0.06013	0.16219
10.5	0.24011	1.03168	0.00159	0.16192	0.22304	1.07162	0.0465	0.15942
11	0.22952	0.98476	0.00153	0.16	0.21388	1.02031	0.03645	0.15598
11.5	0.22111	0.9412	0.00146	0.15759	0.20711	0.97165	0.02905	0.14971
12	0.21018	0.89644	0.00138	0.15537	0.19596	0.92723	0.02244	0.15069
12.5	0.20523	0.85893	0.00132	0.14945	0.19126	0.88804	0.01829	0.14589
13	0.19753	0.82789	0.00126	0.14904	0.18531	0.85258	0.01495	0.14282
13.5	0.19075	0.79665	0.00119	0.14576	0.18038	0.81876	0.01224	0.13938
14	0.18396	0.76897	0.00112	0.14322	0.17297	0.79139	0.01001	0.14118
14.5	0.17688	0.74415	0.00105	0.14153	0.16767	0.76364	0.00825	0.13957
15	0.16894	0.72731	9.93E-04	0.14617	0.16021	0.75247	0.00698	0.15401
15.5	0.1619	0.70584	9.22E-04	0.14555	0.15607	0.72576	0.00578	0.15084
16	0.15866	0.68188	8.63E-04	0.14006	0.15304	0.70019	0.00482	0.14714
16.5	0.15206	0.66323	7.94E-04	0.13944	0.14836	0.67825	0.00399	0.14844

17	0.14804	0.64342	7.38E-04	0.13661	0.14375	0.65965	0.00333	0.15053
17.5	0.14002	0.62946	6.74E-04	0.13676	0.13975	0.63971	0.00277	0.15008
18	0.13722	0.61076	6.20E-04	0.13471	0.13627	0.62221	0.00231	0.15101
18.5	0.13175	0.59575	5.65E-04	0.1322	0.13192	0.60546	0.00191	0.1526
19	0.13031	0.57812	5.18E-04	0.12765	0.12969	0.58804	0.00159	0.15235
19.5	0.12146	0.56907	4.64E-04	0.12989	0.1258	0.57382	0.00132	0.15312
20	0.12235	0.55049	4.24E-04	0.12415	0.12122	0.5611	0.00109	0.15746
20.5	0.11669	0.53921	3.79E-04	0.12348	0.12052	0.54444	9.08E-04	0.15679
21	0.10966	0.53023	3.37E-04	0.12481	0.1187	0.531	7.56E-04	0.1558
21.5	0.1038	0.52179	2.97E-04	0.1275	0.11648	0.51706	6.27E-04	0.1523
22	0.11053	0.50026	2.72E-04	0.1176	0.11059	0.50926	5.14E-04	0.15559
22.5	0.09969	0.49757	2.37E-04	0.12018	0.11243	0.49313	4.32E-04	0.15306
23	0.09436	0.49061	2.05E-04	0.12538	0.10904	0.48286	3.57E-04	0.1497
23.5	0.09427	0.47787	1.84E-04	0.11958	0.10852	0.47109	2.99E-04	0.14612
24	0.10138	0.45879	1.68E-04	0.10465	0.12113	0.44509	2.66E-04	0.12073
24.5	0.09228	0.45671	1.43E-04	0.11057	0.12126	0.43366	2.23E-04	0.11779
25	0.08711	0.45062	1.23E-04	0.10789	0.12273	0.4204	1.88E-04	0.10598
25.5	0.09353	0.43351	1.11E-04	0.09625	0.13103	0.40129	1.61E-04	0.09368
26	0.09159	0.42541	9.59E-05	0.09297	0.13098	0.39136	1.38E-04	0.08667
26.5	0.10156	0.40579	8.65E-05	0.0839	0.13671	0.3756	1.19E-04	0.07067
27	0.10761	0.3902	7.73E-05	0.06207	0.12376	0.3787	9.71E-05	0.06948
27.5	0.10778	0.38084	6.80E-05	0.0602	0.18502	0.30806	1.04E-04	0.01984
28	0.08624	0.39399	5.35E-05	0.07105	0.16619	0.31839	8.39E-05	0.02288
28.5	0.09526	0.37677	4.86E-05	0.04777	0.14226	0.33418	6.33E-05	0.03457
29	0.1288	0.33515	4.65E-05	0.03678	0.21134	0.25728	7.22E-05	0.00437
29.5	0.08943	0.3666	3.69E-05	0.02926	0.06405	0.39625	3.61E-05	0.03178
30	0.12704	0.32048	3.65E-05	0	0.14033	0.31193	3.99E-05	0

T (K)	$\Delta\chi$ (emu/mol)	τ (s)	α	
	H_{dc} = 1 kOe (HF)			
2	0.87631	0.00413	0.25812	
2.15	0.81867	0.00354	0.26354	
2.4	0.74427	0.00275	0.27353	
2.6	0.69635	0.00223	0.2782	
2.8	0.64725	0.00177	0.27931	
3	0.61528	0.00144	0.29201	
3.2	0.57904	0.00117	0.28984	
3.4	0.55856	9.47E-04	0.29807	
3.6	0.53207	7.73E-04	0.29495	
3.8	0.50001	6.25E-04	0.28965	
4	0.47607	5.38E-04	0.28964	
4.2	0.45863	4.46E-04	0.29349	
4.4	0.44974	3.55E-04	0.3103	
4.6	0.43075	3.01E-04	0.30275	
4.8	0.40954	2.62E-04	0.295	
5	0.39457	2.23E-04	0.29489	

Table S6. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **3** by the single-component generalized Debye model at1000 Oe dc field.

T (K)	χ_S (emu/mol)	$\Delta\chi$ (emu/mol)	τ (s)	α
	H_{dc} = 1 kOe			
2	0.10746	5.32697	0.34292	0.18627
2.15	0.10048	4.95191	0.25997	0.18611
2.4	0.08893	4.45045	0.16697	0.18785
2.6	0.07379	4.0966	0.11314	0.19531
2.8	0.06206	3.82027	0.07884	0.20281
3	0.05319	3.5693	0.05493	0.21061
3.2	0.04009	3.37359	0.03927	0.2202
3.4	0.03246	3.19279	0.02835	0.22795
3.6	0.01985	3.02637	0.02046	0.23355
3.8	0.0152	2.87603	0.01526	0.2376
4	0.00564	2.74015	0.01146	0.24202
4.2	3.84E-04	2.62054	0.00881	0.24568
4.4	0	2.50256	0.00683	0.24523
4.6	0	2.39855	0.00542	0.24574
4.8	0	2.29935	0.00431	0.24608
5	0	2.21131	0.00347	0.24656
5.5	0	2.01504	0.00211	0.24769
6	0	1.85001	0.00133	0.2481
6.5	0	1.71453	8.81E-04	0.24833
7	0	1.59593	5.96E-04	0.2506
7.5	0	1.49441	4.11E-04	0.25587
8	0	1.403	2.84E-04	0.25859
8.5	0	1.32293	1.99E-04	0.26004
9	0	1.25047	1.40E-04	0.26122
9.5	0	1.18624	1.00E-04	0.26003
10	0.03374	1.09263	7.62E-05	0.24948

Table S7. CASSCF energies (cm^{-1}) and g-factors for the first eight Kramers' doublets of **1**−**3**.

Molecule	KD	E (cm^{-1})	g_x	g_y	g_z
1	1	0.0	0.006225	0.007459	19.618221
	2	194.5	0.116942	0.202182	16.698357
	3	245.9	0.090887	0.214980	19.086078
	4	317.1	0.154904	0.794469	12.160257
	5	368.6	1.240526	2.281376	13.009951
	6	409.5	1.591427	4.670779	10.034933
	7	470.9	2.203363	4.174282	14.756280
	8	609.3	0.173917	0.426065	19.020685
2	1	0.0	0.002126	0.003183	19.749982
	2	205.8	0.033876	0.047223	17.162357
	3	342.9	0.259272	0.422072	14.130687
	4	423.3	1.000680	1.782779	11.741771
	5	481.8	1.581204	1.751083	15.987122
	6	529.0	0.385897	6.259126	7.333016
	7	610.9	2.514319	4.100738	13.269452
	8	718.9	0.384544	1.345818	18.206785
3	1	0.0	0.018641	0.031649	19.540294
	2	150.0	0.594557	1.260470	15.468396
	3	199.1	0.294455	1.350715	14.300613
	4	280.9	0.823840	2.522789	12.922492
	5	353.6	1.322978	4.827725	9.653844
	6	444.5	2.366021	5.409026	9.435083
	7	553.3	1.597940	2.503451	12.356695
	8	635.8	0.602097	2.466061	17.103471

Table S8. Structural and magnetic features of linear trinuclear Zn-Dy-Zn complexes with salen-type compartmental Schiff base ligands.[a]

Complex	Ln center geometry	Field (Oe)	U_{eff}/K	t_0 (s)	Ref.
$[Dy\{Zn(L^1)(AcO)\}_2]BPh_4$	deca-coordination	1000	22.4	5.3×10^{-7}	60
$[(L^2Zn(H_2O))_2Dy(H_2O)](CF_3SO_3)_3$	MFF-9 (C_s)	0 1000	96.9 128.6	2.4×10^{-4} 1.8×10^{-8}	61
$[(L^2ZnBr)_2Dy(H_2O)](ClO_4)$	TCTPR-9 (D_{3h})	0 1000	146.8) 214.7	9.2×10^{-8} 9.8×10^{-9}	61
$[(L^2ZnCl)_2Dy(H_2O)](ClO_4)(MeOH)$	TCTPR-9 (D_{3h})	0 1000	146.1 202.4	9.9×10^{-8} 1.5×10^{-8}	61
$[Dy(ZnL^3)_2(CH_3COO)Cl_2]\cdot CH_2Cl_2$	TDD-8 (D_{2d}), SAPR-8 (D_{4d})	700	19	1.5×10^{-5}	62
$[Zn_2(L^4)_2DyCl_3]\cdot 2H_2O$[b]	CSAPR-9 (C_{4v}), TCTPR-9 (D_{3h}), MFF-9 (C_s)	0 1000	430 481	7.4×10^{-11} 1.3×10^{-11}	63
$[Zn_2(L^4)_2Dy(MeOH)Br_3]\cdot 3H_2O$[b]	CSAPR-9 (C_{4v}), TCTPR9 (C_{4v}), MFF-9 (C_s)	0	233	2.5×10^{-8}	63
$[Zn_2(L^4)_2Dy(H_2O)Br_2]\cdot[ZnBr_4]_{0.5}$[b]	CSAPR-9(C_{4v}), TCTPR9 (C_{4v}), MFF-9 (C_s)	0	121	8.5×10^{-7}	63
$[Zn_2(L^5)_2DyCl_3]\cdot 2H_2O$[b]	CSAPR-9(C_{4v}), TCTPR9 (C_{4v}), MFF-9 (C_s)	0	398	3.5×10^{-10}	63
$[(ZnL^1Cl)_2Dy(H_2O)]_4[ZnCl_4]_2\cdot H_2O$	CSAPR-9 (C_{4v})	0 1000	67.6 90.6	2.0×10^{-6} 2.2×10^{-5}	64
$[Zn_2Dy(R,R\text{-}L^5)_2(H_2O)_4](ClO_4)_3$	CSAPR-9 (C_{4v})	400	22.46	5.06×10^{-6}	65
$[(L^6ZnCl_{0.5}(OH)_{0.5})(L^6ZnCl)Dy(H_2O)](ZnCl_4)_{0.5}$	CSAPR-9 (C_{4v}), JTCTPR-9 (D_{3h}), MFF-9(C_s)	0	250	2.57×10^{-9}	66
$[DyZn_2(L^7)Cl_2(H_2O)](ClO_4)\cdot 0.5MeOH\cdot 0.25H_2O$	MFF-9 (C_s), TCTPR-9 (D_{3h})	1800	212.1	7.0×10^{-10}	67
$[DyZn_2(L^8)Cl_2(H_2O)][DyZn_2(L^8)Cl_2(MeOH)](ClO_4)_2\cdot MeOH\cdot 0.5H_2O$	MFF-9 (C_s), TCTPR-9 (D_{3h})	1800	194.5	3.1×10^{-9}	67
$[DyZn_2(L^7)Cl_2(H_2O)](CF_3SO_3)\cdot 0.5MeOH$	MFF-9 (C_s), TCTPR-9 (D_{3h})	2000	203.5	1.0×10^{-10}	67
$[DyZn_2(L^8)Cl_2(H_2O)]$-$[DyZn_2(L^8)Cl_2(MeOH)](CF_3SO_3)_2\cdot MeOH$	MFF-9 (C_s), TCTPR-9 (D_{3h})	2000	70.1	8.0×10^{-7}	67
$[DyZn_2(L^7)Br_2(H_2O)](CF_3SO_3)\cdot 0.25MeOH$	MFF-9 (C_s), TCTPR-9 (D_{3h})	2000	207.3	1.5×10^{-10}	67
$[DyZn_2(L^8)Br_2(H_2O)][DyZn_2(L^8)Br_2(MeOH)](CF_3SO_3)_2$	MFF-9 (C_s)/ TCTPR-9 (D_{3h})	2000	218.1	3.5×10^{-11}	67
$[Zn_2Dy(L)_2Cl_2(H_2O)](ClO_4)\cdot 4H_2O$ (**1**),	CSAPR-9 (C_{4v}), JTCTPR-9 (D_{3h}), MFF-9(C_s)	0 1000	244 309	4.8×10^{-9} 5.4×10^{-10}	This work
$[Zn_2Dy(L)_2Br_2(H_2O)](ClO_4)\cdot 4H_2O$ (**2**)	CSAPR-9 (C_{4v}), JTCTPR-9 (D_{3h}), MFF-9(C_s)	0 1000	211 269	3.6×10^{-8} 7.7×10^{-9}	This work
$[Zn_2Dy(L)_2(OAc)I(H_2O)]I_3\cdot 4H_2O$ (**3**)	CSAPR-9 (C_{4v}), JTCTPR-9 (D_{3h}), MFF-9(C_s)	1000	72	2.2×10^{-7}	This work

[a] Abbreviations: H_2L^1 = (ethane-1,2-diylbis(azanylylidene))bis(methanylylidene))bis(2-methoxyphenol); H_2L^2 = (2,2-dimethylpropane-1,3-diyl)bis(azanylylidene))bis(methanylylidene))bis(2-methoxy-4-methylphenol); H_2L^3 = *N*,*N*-bis(3-ethoxysalicylidene)phenylene-1,2-diamine; H_2L^4 = 1,2-phenylenebis(azanylylidene))bis(methanylylidene))bis(2-methoxy-4-methylphenol); H_2L^5 = cyclohexane-1,2-diyl)bis(azanylylidene))bis(methanylylidene))bis(2-methoxy-4-methylphenol); H_2L^6 = *N, N*'-bis(3-methoxysalicylaldiimine)-1,3-propylene-2-ol; H_2L^7 = 2-((*E*)-((1*R*,2*R*)-2-((*E*)-2-hydroxy-3-methoxybenzylideneamino)cyclohexylimino)methyl)-6-methoxyphenol; H_2L^8 = 2-((*E*)-((1*S*,2*S*)-2-((*E*)-2-hydroxy-3-methoxybenzylideneamino)cyclohexylimino)methyl)-6-methoxyphenol; MFF-9 = Muffin; TCTPR-9 = Spherical tricapped trigonal prism; CSAPR-9 = Spherical capped square antiprism; JTCTPR-9 = Tricapped trigonal prism J51. [b] purely Arrhenius law was applied.