Supplementary Information

Influence of Anion Induced Geometrical Change in Zn(II) on Magnetization Relaxation Dynamics of Dy(III) in Zn-Dy-Zn complexes

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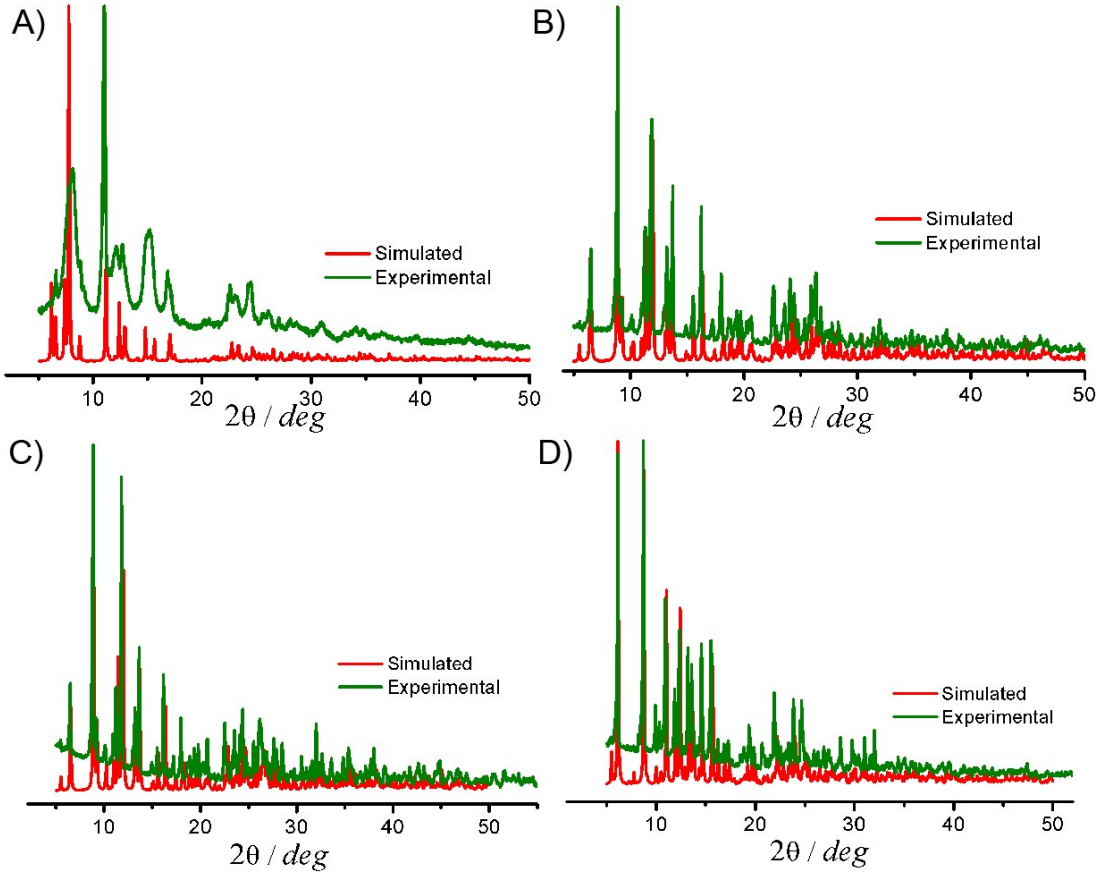

Figure S1. Powder X-ray diffraction pattern of complexes **1-4** (panel A-D).

Table S1. Shape measurement of Dy(III) center of complexes **1-4**

S.No.	Geometry	Point group	Deviation from the indicated geometry				
			Complex **1**	Complex **2**	Complex **3**	Complex **4**	
						4a	**4b**
1	Octagon	D_{8h}	30.464	29.743	29.729	30.216	30.085
2	Heptagonal pyramid	C_{7v}	23.274	23.373	23.319	22.724	23.053
3	Hexagonal bipyramid	D_{6h}	16.031	15.979	15.867	16.103	17.063
4	Cube	O_h	9.998	9.553	9.495	10.123	9.827
5	Square antiprism	D_{4d}	**0.494**	**0.523**	**0.501**	**0.460**	**0.452**
6	Triangular dodecahedron	D_{2d}	2.655	2.602	2.598	2.575	2.595
7	Johnson gyrobifastigiumJ26	D_{2d}	15.328	15.804	15.714	15.416	15.942
8	Johnson elongated triangular bipyramid J14	D_{3h}	28.112	28.062	27.992	28.233	28.352
9	Biaugmented trigonal prism J50	C_{2v}	2.675	2.641	2.628	2.799	2.825
10	Biaugmented trigonal prism	C_{2v}	2.372	2.315	2.306	2.493	2.494
11	Snub diphenoid J84	D_{2d}	4.811	4.886	4.879	5.073	4.930
12	Triakis tetrahedron	T_d	10.788	10.088	10.023	10.941	10.398
13	Elongated trigonal bipyramid	D_{3h}	23.608	23.901	23.857	23.708	23.975

Table S2 Shape measurement of Zn(II) centers of complexes **1-4**

S.No.	Geometry of **Zn1/Zn2**	Point group	**1**	**2**	**3**	**4**	
						4a	**4b**
1	Pentagon	D_{5h}	33.37/33.63	31.69/31.08	31.56/30.96	31.66/30.40	31.33/30.41
2	Vacant octahedron	C_{4v}	4.97/4.02	2.59/3.00	2.53/2.94	3.18/4.67	4.47/3.10
3	Trigonal bipyramid	D_{3h}	**1.48/2.33**	4.63/3.26	**1.785/2.33**	2.93/**2.14**	**2.14**/3.81
4	Spherical square pyramid	C_{4v}	3.25/2.35	**1.16/1.67**	2.96/2.34	**1.60**/2.96	2.78/**1.43**
5	Johnson trigonal bipyramid J12	D_{3h}	2.69/3.26	5.62/4.60	5.80/4.64	4.30/3.26	3.16/5.02
Angular structural indices (τ) for five coordinate Zn(II) ion							
τ	Zn1/Zn2		0.77/0.70	0.23/0.40	0.55/0.52	0.39/0.71	0.71/0.30

Table S3. Selected bond length (Å) and bond angle (°)for complexes **1-4**

Label	1	2	3	4	
				4a	4b
Dy-O11	2.35(3)	2.35(1)	2.31(3)	2.31(4)	2.33(4)
Dy-O12	2.55(3)	2.52(1)	2.51(3)	2.50(3)	2.52(4)
Dy-O31	2.34(3)	2.35(2)	2.35(8)	2.34(4)	2.30(4)
Dy-O32	2.52(3)	2.55(1)	2.46(10)	2.53(4)	2.50(4)
Dy-O52	2.28(1)	2.31(3)	2.28(4)	2.30(4)	2.30(3)
Dy-O53	2.28(1)	2.27(2)	2.27(4)	2.29(4)	2.32(4)
Dy-O56	2.28(2)	2.28(3)	2.27(3)	2.30(3)	2.27(4)
Dy-O57	2.28(2)	2.28(2)	2.28(3)	2.28(4)	2.30(4)
Zn1-O31	2.02(3)	2.02(2)	2.07(8)	2.02(4)	2.04(4)
Zn1-O33	2.30(4)	2.40(3)	2.30(9)	2.32(4)	2.38(4)
Zn1-N31	2.04(4)	2.02(3)	2.11(10)	2.02(4)	2.01(4)
Zn1-O51	1.94(1)	1.95(3)	1.94(4)	1.96(4)	1.96(4)
Zn1-O55	1.94(1)	1.97(3)	1.94(4)	1.97(4)	1.97(4)
Zn2-O11	2.02(3)	2.02(2)	2.03(3)	2.04(4)	2.03(4)
Zn2-O13	2.40(4)	2.30(3)	2.35(4)	2.35(4)	2.36(4)
Zn2-N11	2.01(4)	2.03(3)	1.98(5)	2.00(4)	2.02(4)
Zn2-O54	1.93(1)	1.97(3)	1.93(4)	1.96(4)	1.96(4)
Zn2-O58	1.95(1)	1.96(3)	1.95(3)	1.96(4)	1.97(3)
BondAngle(°)					
Dy-O31-Zn1	112.22(12)	111.69(10)	109.02(4)	111.13(2)	110.52(2)
Dy-O11-Zn2	111.67(12)	111.67(12)	112.8(4)	111.12(2)	111.31(2)
Zn1-Dy-Zn2	175.57(1)	175.59(1)	171.51(3)	168.76(1)	171.81(1)

Table S4. Atoms involved in the intermolecular hydrogen bonding for complexes **1**-4

Complex **1**

Hydrogen bonds for zndy [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17A)...O(2A^b)#1	0.95	2.51	3.452(11)	170.1
C(19)-H(19A)...O(3^a)#1	0.95	2.61	3.506(13)	157.3
C(19)-H(19A)...Br(1^d)	0.95	2.89	3.731(5)	148.2
C(22)-H(22A)...O(2A^b)#2	0.95	2.58	3.482(11)	159.0
C(22)-H(22A)...O(3B^c)#2	0.95	2.57	3.501(16)	165.8
C(24)-H(24A)...O(3B^c)#2	0.98	2.66	3.175(17)	113.0
C(24)-H(24C)...O(62)	0.98	2.64	3.199(7)	116.6

C(25)-H(25B)...O(81)	0.98	2.51	3.085(6)	117.2
C(33)-H(33A)...O(2^a)	0.95	2.39	3.327(10)	169.5
C(33)-H(33A)...O(2^a)#1	0.95	2.63	3.576(11)	173.3
C(37)-H(37A)...O(2B^c)#3	0.95	2.64	3.397(15)	136.7
C(39)-H(39A)...O(2B^c)#3	0.95	2.52	3.464(14)	176.0
C(44)-H(44C)...O(72)	0.98	2.61	3.158(7)	115.8
C(45)-H(45B)...O(51)	0.98	2.53	3.082(6)	115.3
C(45)-H(45C)...O(2^a)	0.98	2.58	3.412(11)	142.3
C(82)-H(82B)...O(1A^b)#4	0.98	2.58	3.548(11)	171.9
C(82)-H(82C)...O(52)#3	0.98	2.57	3.439(6)	147.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y,-z+1 #2 x,-y+3/2,z-1/2 #3 x+1/2,-y+1,z
#4 x+1/2,y-1/2,z-1/2

Complex **2**

Hydrogen bonds for dyzn [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(13)-H(13A)...O(4^a)	0.95	2.33	3.231(9)	159.1
C(13)-H(13A)...O(4A^b)	0.95	2.62	3.562(15)	171.1
C(13)-H(13A)...O(4A^b)#1	0.95	2.33	3.270(11)	171.5
C(17)-H(17A)...O(5^a)	0.95	2.64	3.434(9)	141.5
C(19)-H(19A)...O(5^a)	0.95	2.59	3.531(9)	171.0
C(19)-H(19A)...O(8A^b)	0.95	2.55	3.498(19)	174.9
C(24)-H(24A)...O(56)	0.98	2.61	3.161(5)	115.4
C(24)-H(24B)...O(6A^b)#2	0.98	2.53	3.50(2)	171.4
C(25)-H(25A)...O(53)	0.98	2.54	3.096(5)	116.1
C(25)-H(25C)...O(3^a)#1	0.98	2.66	3.606(11)	162.6
C(25)-H(25C)...O(4^a)	0.98	2.52	3.395(12)	148.6
C(25)-H(25C)...O(3A^b)#1	0.98	2.63	3.318(19)	127.6
C(25)-H(25C)...O(4A^b)#1	0.98	2.54	3.334(19)	137.6
C(33)-H(33A)...O(3^a)#3	0.95	2.52	3.218(10)	129.9
C(33)-H(33A)...O(1A^b)#3	0.95	2.49	3.416(16)	166.5
C(37)-H(37A)...O(5B^c)#4	0.95	2.63	3.568(12)	171.0
C(39)-H(39A)...O(1^a)	0.95	2.57	3.460(10)	155.6
C(39)-H(39A)...O(2^a)#1	0.95	2.53	3.409(9)	154.8

C(39)-H(39A)...O(3A^b)#1	0.95	2.53	3.393(14)	150.6
C(44)-H(44A)...O(52)	0.98	2.62	3.189(5)	117.1
C(44)-H(44B)...O(6B^c)#5	0.98	2.26	2.926(16)	124.2
C(44)-H(44C)...O(6B^c)#6	0.98	2.24	2.789(14)	114.1
C(45)-H(45A)...O(57)	0.98	2.49	3.073(5)	117.8
C(54)-H(54A)...O(57)#7	0.98	2.44	3.353(5)	154.8
C(58)-H(58A)...O(7B^c)#2	0.98	2.61	3.542(18)	159.7
C(58)-H(58C)...O(54)#3	0.98	2.56	3.471(4)	155.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y,-z+2 #2 x,-y+3/2,z-1/2 #3 x+1/2,-y+2,z

#4 -x+2,-y+2,-z+2 #5 x-1/2,y+1/2,z-1/2 #6 -x+2,y+1/2,-z+3/2

#7 x-1/2,-y+2,z

Complex **3**

Hydrogen bonds for zndy_sq [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17)...Cl(1A)#1	0.95	2.50	3.436(14)	170.4
C(19)-H(19)...Cl(1A)#1	0.95	2.86	3.484(15)	124.2
C(19)-H(19)...Cl(1A)#2	0.95	2.95	3.811(12)	151.9
C(24)-H(24A)...O(54)	0.98	2.67	3.214(8)	115.6
C(24)-H(24C)...O(33^a)#1	0.98	2.61	3.331(16)	130.8
C(24)-H(24C)...O(33A^b)#1	0.98	2.54	3.331(15)	138.1
C(25)-H(25A)...O(31A^b)	0.98	2.51	3.093(19)	118.0
C(37^a)-H(37A^a)...Cl(1A)	0.95	2.82	3.714(16)	156.8
C(39^a)-H(39A^a)...Cl(1)	0.95	2.85	3.778(11)	164.4
C(45^a)-H(45C^a)...O(57)	0.98	2.67	3.133(17)	109.4
C(58)-H(58C)...O(57)#3	0.98	2.57	3.520(7)	162.0

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 -x+1,-y+1,-z+1 #3 -x,-y+1,-z+1

Complex **4**

Hydrogen bonds for dyzn [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(22)-H(22A)...F(12^a)#1	0.95	2.63	3.571(10)	169.4
C(22)-H(22A)...F(13A^b)#1	0.95	2.40	3.29(2)	157.5
C(24)-H(24B)...F(15^a)#1	0.98	2.60	3.494(10)	151.6
C(24)-H(24B)...F(12A^b)#1	0.98	2.38	3.20(2)	140.7
C(25)-H(25A)...O(31)	0.98	2.66	3.197(7)	114.9
C(39)-H(39A)...O(1W^b)#2	0.95	2.49	3.32(2)	146.2
C(44)-H(44A)...O(55)	0.98	2.66	3.213(8)	116.2
C(45)-H(45A)...O(57)	0.98	2.61	3.165(7)	115.9
C(54)-H(54A)...O(57)#1	0.98	2.35	3.317(8)	169.3
C(56)-H(56C)...O(56)#3	0.98	2.59	3.324(7)	132.1
C(122)-H(12F)...F(22^a)#4	0.95	2.59	3.475(13)	155.4
C(122)-H(12F)...F(25A^b)#4	0.95	2.46	3.343(13)	154.7
C(124)-H(12H)...O(1W^b)	0.98	2.63	3.50(3)	148.0
C(124)-H(12I)...F(26^a)#4	0.98	2.55	3.156(14)	119.9
C(125)-H(12A)...O(152)	0.98	2.61	3.173(7)	116.4
C(125)-H(12C)...F(11^a)#5	0.98	2.63	3.216(9)	118.8
C(125)-H(12C)...F(14A^b)#5	0.98	2.57	3.41(3)	143.7
C(133)-H(13D)...F(14A^b)#6	0.95	2.57	3.26(3)	130.1
C(139)-H(13F)...F(11A^b)#5	0.95	2.58	3.43(2)	149.0
C(142)-H(14E)...F(24^a)#7	0.95	2.63	3.275(11)	125.4
C(145)-H(14B)...O(157)	0.98	2.57	3.096(7)	113.7
C(145)-H(14C)...F(15A^b)#6	0.98	2.55	3.073(15)	113.5
C(156)-H(15K)...O(152)#1	0.98	2.47	3.368(7)	151.5
O(1S^b)-H(11S^b)...F(15A^b)#8	0.84	2.23	3.02(3)	156.0
O(2S^a)-H(2S^a)...F(22^a)#4	0.84	2.60	3.32(2)	144.6
C(21S^a)-H(21C^a)...F(25^a)	0.99	2.32	3.17(2)	142.2

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x+1,-y+1,-z+2 #3 -x+2,-y+2,-z+2

#4 x-1,y,z #5 -x,-y+1,-z+1 #6 x,y-1,z #7 -x+1,-y+1,-z+1
#8 x+1,y-1,z

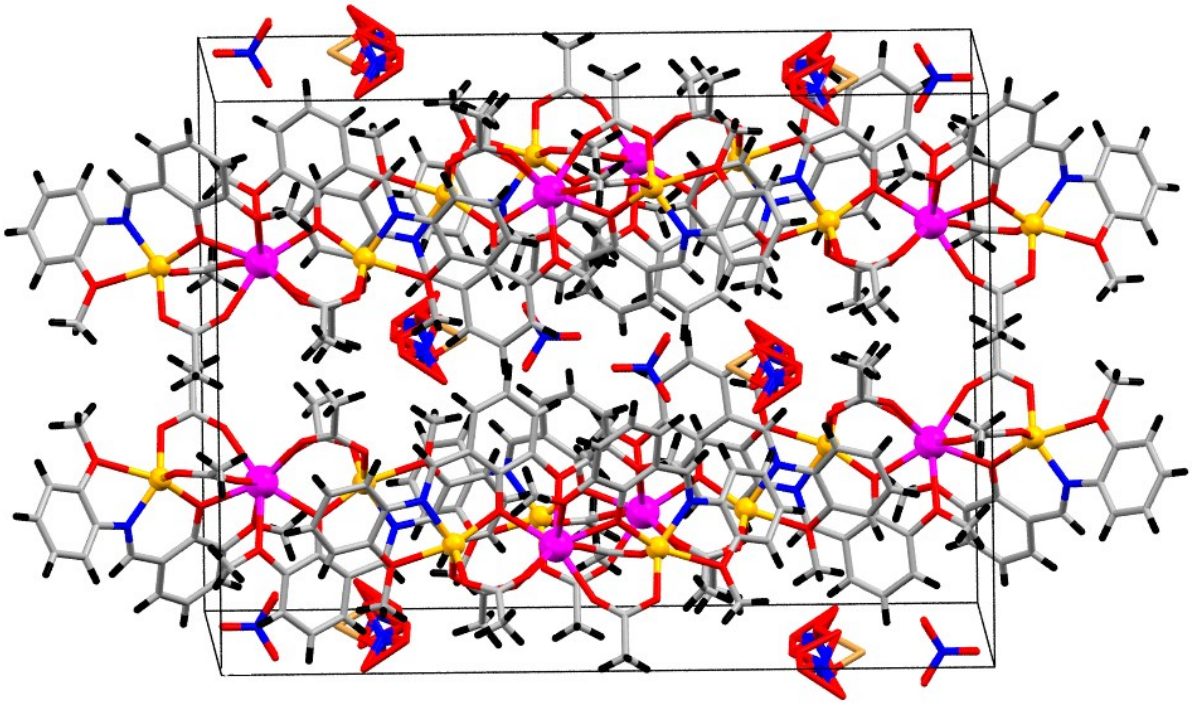

Figure S2. Packing diagram of complexes **1**. The closest Ln---Ln distance is 8.53 Å

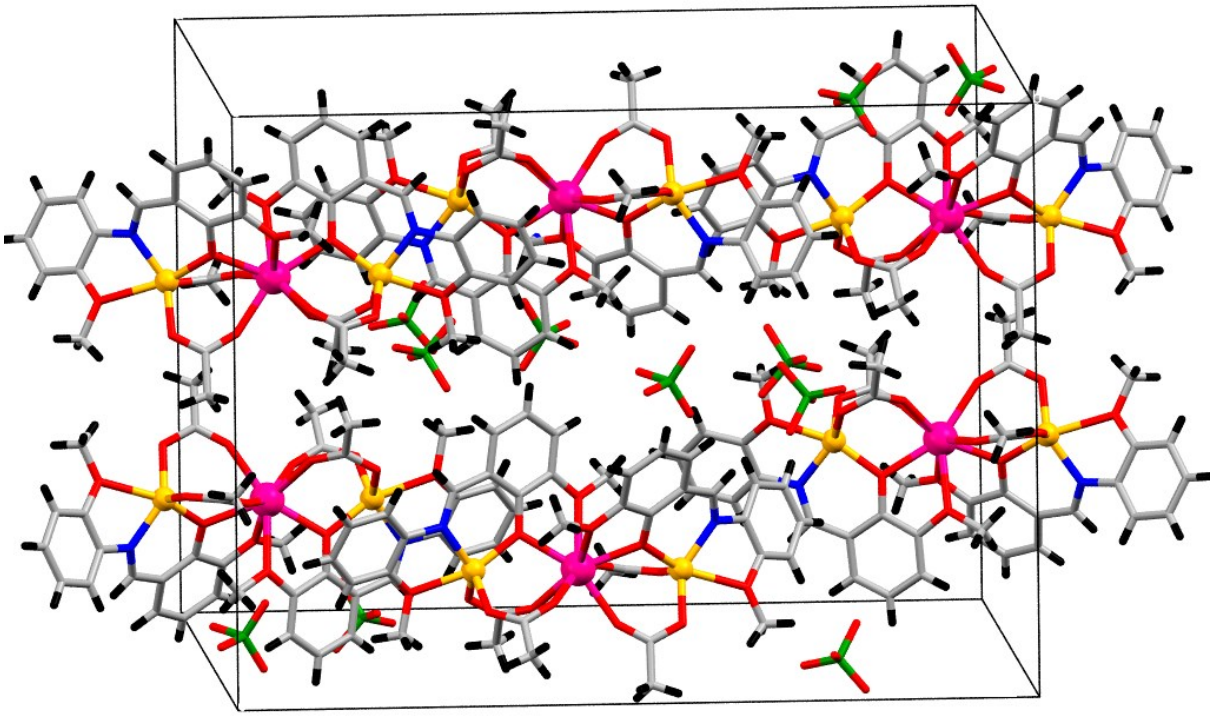

Figure S3. Packing diagram of complexes **2**. The closest Ln---Ln distance is 8.56 Å

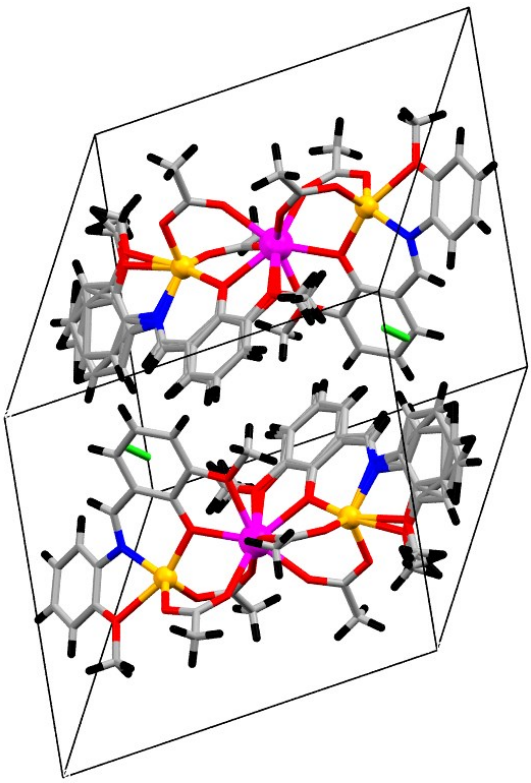

Figure S4. Packing diagram of complexes **3**. The closest Ln---Ln distance is 11.06 Å

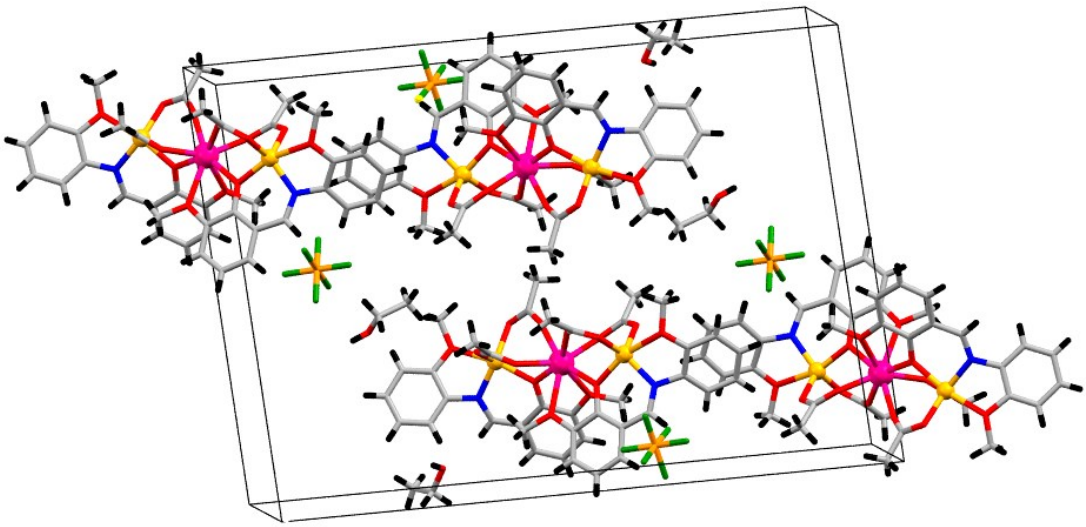

Figure S5. Packing diagram of complexes **4**. The closest Ln---Ln distance is 11.4 Å.

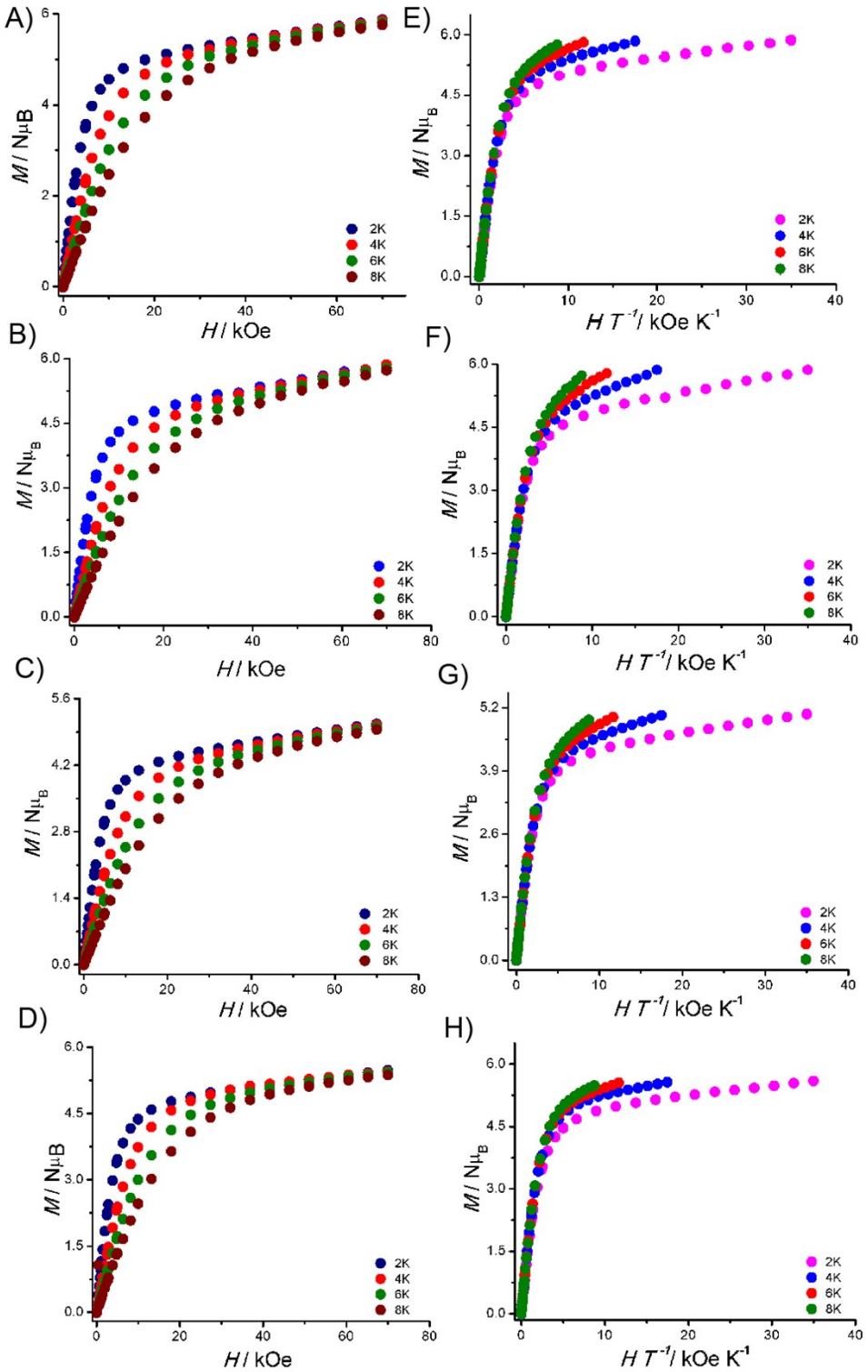

Figure S6. Field dependent magnetization plot (panels A-D) and the reduced magnetization plot(panels E-H) for complexes **1-4**, respectively.

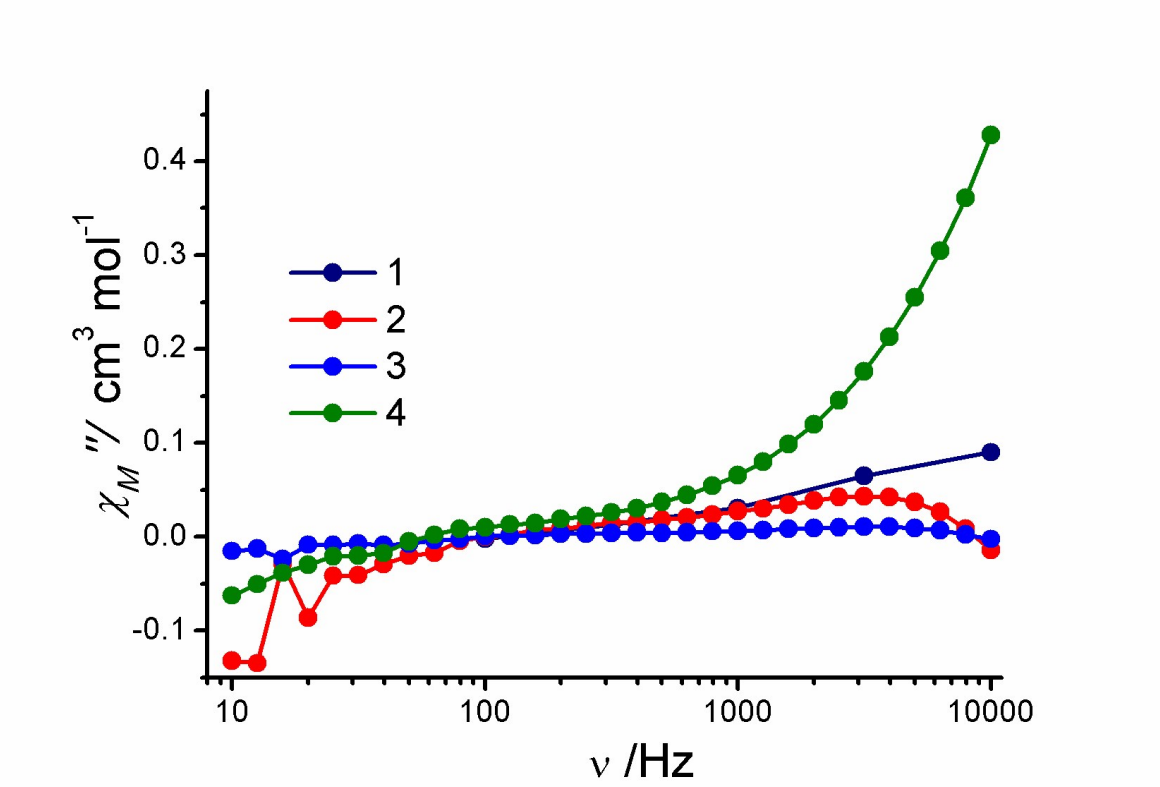

Figure S7. The frequency-dependent out of phase susceptibility measurement done on polycrystalline sample of complex **1-4** in the presence of Zero Oe external magnetic field at 2K.

Table S5. The best fitting parameters obtained for Cole-Cole plot of complex **1**

S.No.	Temp.	χ_S	χ_T	τ	α	Residual
1	2.8	0.984390E+00	0.984390E+00	0.146564E-03	0.629793E+00	0.116123E-01
2	2.9	0.105552E+01	0.273141E+01	0.133776E-03	0.586904E+00	0.166539E-01
3	3	0.110373E+01	0.273967E+01	0.135192E-03	0.557652E+00	0.168313E-01
4	3.1	0.115686E+01	0.273392E+01	0.135873E-03	0.522166E+00	0.273505E-01
5	3.2	0.117741E+01	0.273438E+01	0.132078E-03	0.500176E+00	0.122074E-01
6	3.3	0.121177E+01	0.272181E+01	0.130241E-03	0.469070E+00	0.144872E-01
7	3.4	0.120570E+0	0.270864E+01	0.120672E-03	0.458049E+00	0.326749E-01
8	3.5	0.123745E+01	0.269853E+01	0.122296E-03	0.428428E+00	0.101602E-01
9	3.6	0.126016E+01	0.267380E+01	0.119621E-03	0.398487E+00	0.840707E-02
10	3.7	0.124507E+01	0.266407E+01	0.112710E-03	0.395080E+00	0.176214E-01
11	3.8	0.125507E+01	0.265074E+01	0.111553E-03	0.376303E+00	0.111982E-01
12	3.9	0.124981E+01	0.262747E+01	0.106141E-03	0.364482E+00	0.180647E-01
13	4	0.125796E+01	0.259629E+01	0.102313E-03	0.341563E+00	0.836806E-02
14	4.1	0.125624E+01	0.257639E+01	0.987504E-04	0.328052E+00	0.147613E-01
15	4.2	0.124310E+01	0.255236E+01	0.929399E-04	0.321366E+00	0.294591E-01
16	4.3	0.124243E+01	0.252867E+01	0.895215E-04	0.307151E+00	0.149736E-01
17	4.4	0.124594E+01	0.248011E+01	0.834203E-04	0.280436E+00	0.150738E-01
18	4.5	0.123650E+01	0.245827E+01	0.791588E-04	0.272522E+00	0.189915E-01
19	4.6	0.122292E+01	0.244015E+01	0.750235E-04	0.269698E+00	0.147786E-01
20	4.8	0.120940E+01	0.237762E+01	0.656158E-04	0.245016E+00	0.184410E-01
21	5	0.120410E+01	0.230441E+01	0.567174E-04	0.208940E+00	0.269986E-01
22	5.2	0.118021E+01	0.225459E+01	0.485070E-04	0.199261E+00	0.275633E-01
23	5.4	0.116503E+01	0.219820E+01	0.411502E-04	0.181589E+00	0.141092E-01
24	5.6	0.113594E+01	0.215679E+01	0.344894E-04	0.184908E+00	0.692663E-02
25	5.8	0.113131E+01	0.210118E+01	0.291748E-04	0.162506E+00	0.118453E-01
26	6	0.112579E+01	0.204822E+01	0.244248E-04	0.147127E+00	0.128547E-01
27	6.2	0.113261E+01	0.199209E+01	0.207799E-04	0.118662E+00	0.946012E-02
28	6.4	0.109911E+01	0.195662E+01	0.165806E-04	0.136583E+00	0.999380E-02
29	6.6	0.109147E+01	0.191025E+01	0.136827E-04	0.129156E+00	0.795555E-02
30	6.8	0.109086E+01	0.185975E+01	0.114028E-04	0.107115E+00	0.111327E-01
31	7	0.108584E+01	0.182170E+01	0.940096E-05	0.116005E+00	0.806694E-02

Table S6. The best fitting parameters obtained for the Cole-Cole plot of complex **2**

S.No.	Temperature	χ_S	χ_T	τ	α	Residual
1	2.2	0.221174E+00	0.334452E+01	0.230288E-04	0.256375E+00	0.229323E-01
2	2.3	0.242764E+00	0.332580E+01	0.179709E-04	0.235447E+00	0.219876E-01
3	2.4	0.260019E+00	0.329933E+01	0.140629E-04	0.214854E+00	0.214273E-01
4	2.5	0.219371E+00	0.326975E+01	0.107062E-04	0.203340E+00	0.173839E-01
5	2.6	0.148280E+00	0.323321E+01	0.808120E-05	0.195422E+00	0.144842E-01
6	2.7	0.877145E-02	0.319364E+01	0.594342E-05	0.194428E+00	0.110009E-01
7	2.8	0.432373E+00	0.314223E+01	0.612796E-05	0.161865E+00	0.124419E-01
8	2.9	0.588761E-14	0.309827E+01	0.377626E-05	0.185655E+00	0.648379E-02
9	3	0.310567E-13	0.304440E+01	0.306475E-05	0.183048E+00	0.408532E-02
10	3.1	0.417962E-13	0.299059E+01	0.246415E-05	0.188453E+00	0.323860E-02
11	3.2	0.915205E-07	0.293399E+01	0.199290E-05	0.194612E+00	0.203322E-02
12	3.3	0.672974E-05	0.287809E+01	0.161056E-05	0.204358E+00	0.155219E-02
13	3.4	0.209504E-13	0.281837E+01	0.138956E-05	0.197238E+00	0.136120E-02
14	3.5	0.451281E-13	0.276437E+01	0.106362E-05	0.225351E+00	0.596627E-03
15	3.6	0.171872E-05	0.270933E+01	0.863249E-06	0.238155E+00	0.757305E-03

Table S7. The best fitting parameters obtained for the Cole-Cole plot of complex **3**

S.No.	Temperature	χ_S	χ_T	τ	α	Residual
1	2.2	0.626407E+00	0.312006E+01	0.130256E-03	0.209284E+00	0.445914E-01
2	2.3	0.603551E+00	0.307893E+01	0.106083E-03	0.206232E+00	0.307652E-01
3	2.4	0.582980E+00	0.303171E+01	0.856370E-04	0.201759E+00	0.267337E-01
4	2.5	0.570619E+00	0.297901E+01	0.688335E-04	0.193810E+00	0.167141E-01
5	2.6	0.565944E+00	0.292104E+01	0.554933E-04	0.182707E+00	0.108180E-01
6	2.7	0.553837E+00	0.287059E+01	0.447810E-04	0.177643E+00	0.154577E-01
7	2.8	0.557689E+00	0.557689E+00	0.365343E-04	0.167447E+00	0.983630E-02
8	2.9	0.558255E+00	0.276264E+01	0.299059E-04	0.160771E+00	0.999251E-02
9	3	0.600333E+00	0.270361E+01	0.251168E-04	0.147153E+00	0.741668E-02
10	3.1	0.568217E+00	0.264869E+01	0.201843E-04	0.147424E+00	0.204979E-01
11	3.2	0.646770E+00	0.258190E+01	0.177831E-04	0.118333E+00	0.107985E-01
12	3.3	0.636818E+00	0.253639E+01	0.147081E-04	0.123705E+00	0.582840E-02
13	3.4	0.615343E+00	0.249209E+01	0.119677E-04	0.135181E+00	0.115405E-01
14	3.5	0.647802E+00	0.244033E+01	0.104427E-04	0.127112E+00	0.792144E-02
15	3.6	0.659235E+00	0.238921E+01	0.885157E-05	0.127431E+00	0.607193E-02
16	3.7	0.654605E+00	0.233779E+01	0.736505E-05	0.132141E+00	0.649278E-02
17	3.8	0.705382E+00	0.229029E+01	0.661401E-05	0.125077E+00	0.491642E-02
18	3.9	0.643420E+00	0.224425E+01	0.526789E-05	0.137442E+00	0.481929E-02
19	4	0.731279E+00	0.219787E+01	0.486062E-05	0.131480E+00	0.580935E-02

Table S8. The best fitting parameters obtained for the Cole-Cole plot of complex **4**

S.No.	Temperature	χ_S	χ_T	τ	α	Residual
1	2.3	0.316575E+00	0.122355E+02	0.961912E+00	0.461605E+00	0.185537E-01
2	2.6	0.312412E+00	0.516639E+01	0.762250E-01	0.357744E+00	0.188478E-01
3	3.2	0.291468E+00	0.318557E+01	0.113516E-01	0.203802E+00	0.234780E-01
4	3.8	0.264074E+00	0.259477E+01	0.350438E-02	0.116593E+00	0.263477E-01
5	4	0.249326E+00	0.240364E+01	0.211940E-02	0.952194E-01	0.233251E-01
6	4.4	0.234607E+00	0.225319E+01	0.133476E-02	0.848015E-01	0.173011E-01
7	4.7	0.221284E+00	0.211212E+01	0.853938E-03	0.773325E-01	0.128383E-01
8	5	0.211040E+00	0.198443E+01	0.559155E-03	0.695435E-01	0.129567E-01
9	5.3	0.200000E+00	0.188593E+01	0.375941E-03	0.716411E-01	0.751822E-02
10	5.6	0.194289E+00	0.178269E+01	0.253720E-03	0.673390E-01	0.108651E-01
11	6	0.188669E+00	0.169342E+01	0.173491E-03	0.681587E-01	0.811428E-02
12	6.2	0.187093E+00	0.161204E+01	0.119851E-03	0.687476E-01	0.818423E-02
13	6.5	0.189997E+00	0.154000E+01	0.836391E-04	0.698765E-01	0.859059E-02
14	6.8	0.199388E+00	0.147191E+01	0.589781E-04	0.681127E-01	0.721804E-02
15	7	0.210722E+00	0.141579E+01	0.426185E-04	0.694889E-01	0.640229E-02
16	7.4	0.240494E+00	0.135409E+01	0.315322E-04	0.549226E-01	0.113039E-01
17	7.7	0.261485E+00	0.130621E+01	0.233739E-04	0.540903E-01	0.606618E-02
18	8	0.282790E+00	0.126108E+01	0.173794E-04	0.548378E-01	0.338254E-02
19	8.3	0.314119E+00	0.121365E+01	0.131705E-04	0.456467E-01	0.569606E-02
20	8.6	0.333144E+00	0.117414E+01	0.996858E-05	0.479922E-01	0.388854E-02
21	8.9	0.326394E+00	0.113786E+01	0.723921E-05	0.619144E-01	0.199006E-02
22	9.2	0.331259E+00	0.110314E+01	0.535578E-05	0.727307E-01	0.510258E-02
23	9.5	0.340112E+00	0.106950E+01	0.401326E-05	0.804501E-01	0.235860E-02
24	9.8	0.309091E+00	0.103904E+01	0.277646E-05	0.997683E-01	0.317920E-02

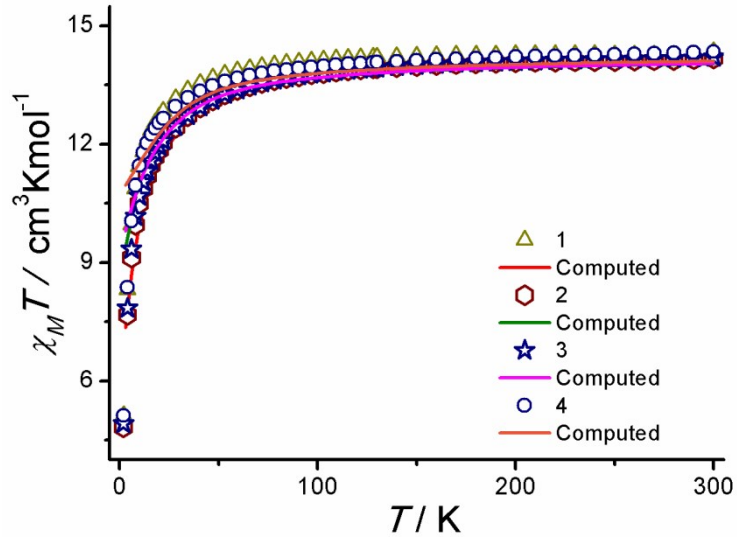

Figure S8. Variable temperature magnetic susceptibility measurement performed on polycrystalline sample of **1-4** in the presence of an applied magnetic field of 10 kOe. The solid trace indicates the computed $\chi_M T$value where the anion is *not* taken into account in the input file.

Table S9. Energies(cm^{-1}) of the low-lying Kramer's doublet for complexes **1-4**, the Computed g-tensors and the angle between the central anisotropic axis and the excited state anisotropic axes of the complexes **1-4**.

Complex 1 $[Zn_2Dy(L_1)_2(OAc)_4].(NO_3)_{0.92}(Br)_{0.08}$									
Without anion					**With anion**				
g_{xx}	**g_{yy}**	**g_{zz}**	**Energy/cm^{-1}**	**θ°**	**g_{xx}**	**g_{yy}**	**g_{zz}**	**Energy/cm^{-1}**	**θ°**
1.23	5.12	12.63	0	0	0.54	1.36	15.52	0	0
1.67	4.45	12.17	15.47	95.81	0.25	2.57	14.94	21.63	87.94
1.55	2.21	13.45	51.21	158.96	0.01	0.99	15.84	50.13	144.64
1.04	2.73	14.28	64.03	146.83	1.61	3.07	11.56	76.58	66.19
4.65	5.46	8.00	89.16	114.89	3.00	4.00	9.13	93.36	104.02
0.10	3.67	12.57	212.86	79.15	0.06	3.76	12.42	213.23	113.79
1.26	2.70	16.19	313.95	78.81	1.29	2.79	16.10	313.82	113.68
0.17	0.55	19.17	458.17	47.07	0.16	0.55	19.17	459.46	45.71
Complex 2 $[Zn_2Dy(L_1)_2(OAc)_4].ClO_4$									
0.32	2.09	16.79	0	0	0.10	1.83	16.89	0	0
0.59	1.18	15.20	19.29	147.71	0.65	0.80	16.04	19.17	32.76

0.40	1.67	15.72	47.32	14.57	0.45	1.47	15.45	46.94	16.33
1.54	2.57	15.20	79.68	126.04	2.05	2.39	15.60	82.50	123.63
7.48	6.88	2.93	111.92	35.36	7.74	6.39	2.51	111.46	37.47
0.65	3.55	12.41	245.83	66.82	0.86	3.57	12.45	240.27	63.57
0.43	2.37	14.63	377.34	70.49	0.73	2.22	15.29	369.32	69.36
0.52	2.37	17.67	464.10	81.57	0.42	1.77	18.16	464.62	86.18
Complex 3 $[Zn_2Dy(L_1)_2(OAc)_4].Cl$									
0.54	2.47	14.01	0	0	0.59	1.55	16.30	0	0
1.06	3.62	12.95	19.42	91.93	1.06	2.75	13.25	30.94	99.81
0.91	3.35	9.02	52.50	142.36	1.59	3.11	10.18	60.74	126.91
1.33	4.26	13.45	78.87	123.35	0.12	4.00	12.02	88.58	123.84
1.12	1.24	15.92	102.40	132.13	1.09	1.88	14.75	103.75	135.96
0.39	3.55	13.21	198.09	75.85	0.59	3.46	13.44	203.07	65.38
1.08	2.35	16.45	297.83	87.06	1.03	2.22	16.55	304.21	45.68
0.12	0.41	19.24	446.69	35.27	0.12	0.37	19.27	456.12	75.99
Complex 4a $[Zn_2Dy(L_1)_2(OAc)_4].PF_6$									
0.13	0.23	18.48	0	0	0.11	0.17	18.57	0	0
1.16	2.53	16.33	42.10	55.77	1.71	4.11	15.09	44.09	47.16
1.23	3.06	14.05	56.71	18.72	2.32	3.92	12.36	56.97	26.70
0.79	2.29	14.93	81.24	21.99	1.14	2.48	15.39	80.53	26.85
7.33	6.36	5.12	121.30	87.52	7.56	6.39	4.76	120.72	61.08
0.78	3.51	12.86	244.06	91.33	0.98	3.50	12.95	237.81	91.85
0.96	2.10	16.26	359.02	90.91	0.99	2.02	16.55	350.19	91.13
0.28	1.00	18.85	469.26	115.63	0.23	0.76	19.01	468.49	116.15
Complex 4b $[Zn_2Dy(L_1)_2(OAc)_4].PF_6$									
0.11	0.27	18.67	0	0	0.13	0.26	18.75	0	0
1.10	2.35	16.03	50.84	39.65	1.82	3.00	15.24	55.47	34.35
0.45	3.58	13.57	70.19	39.83	0.02	3.40	14.38	67.25	34.02
0.43	2.62	15.94	79.91	49.28	0.07	0.51	18.19	86.18	57.71
7.17	6.85	4.51	119.55	72.55	7.4	6.65	4.53	122.48	72.40
1.04	3.48	12.62	245.43	94.25	1.21	3.50	12.60	242.90	93.72
0.76	2.04	15.88	373.23	86.97	0.87	1.99	16.20	367.14	88.03
0.34	1.32	18.59	476.42	125.05	0.28	1.02	18.83	478.38	125.54

Table S10. The computed crystal field parameter for complexes **1-4**where anions are taken into account in the calculations.

B_k^q**parameter**						
K	**q**	**Complex 1**	**Complex 2**	**Complex 3**	**Complex 4a**	**Complex 4b**
2	-2	-0.31	-0.49	0.89	-0.26	-0.42
	-1	-2.43	-1.80	2.17	-3.75	4.91
	0	2.50	-1.64	-0.17	-1.57	-1.25
	1	4.92	-3.32	-3.54	1.60	-1.56
	2	-4.57	-0.55	1.16	0.80×10^{-1}	0.29
4	-4	0.57×10^{-1}	-0.98×10^{-2}	0.18×10^{-1}	0.14×10^{-2}	-0.53×10^{-2}
	-3	-0.97×10^{-1}	-0.97×10^{-2}	-0.70×10^{-2}	0.27×10^{-1}	-0.14×10^{-1}
	-2	-0.50×10^{-1}	0.23×10^{-1}	-0.17×10^{-1}	-0.14×10^{-1}	-0.24×10^{-1}
	-1	-0.15	0.69×10^{-2}	-0.15×10^{-1}	0.21×10^{-1}	-0.14×10^{-1}
	0	0.42×10^{-1}	0.24×10^{-2}	-0.37×10^{-2}	0.12×10^{-2}	-0.36×10^{-3}
	1	0.70×10^{-1}	0.14×10^{-1}	-0.27×10^{-1}	-0.14×10^{-1}	-0.24×10^{-2}
	2	-0.45×10^{-1}	0.18×10^{-2}	0.17×10^{-1}	-0.12×10^{-1}	-0.25×10^{-1}
	3	-0.61	0.33×10^{-1}	-0.66×10^{-1}	-0.10	$0.65\text{x}10^{-1}$
	4	0.22×10^{-1}	0.30×10^{-1}	0.13×10^{-1}	0.76×10^{-3}	-0.28×10^{-2}
6	-6	-0.30×10^{-2}	-0.73×10^{-4}	0.14×10^{-3}	-0.83×10^{-4}	-0.12×10^{-3}
	-5	0.10×10^{-1}	0.19×10^{-3}	0.69×10^{-4}	0.95×10^{-4}	-0.27×10^{-3}
	-4	-0.35×10^{-2}	0.14×10^{-3}	-0.98×10^{-4}	0.21×10^{-3}	0.21×10^{-3}
	-3	0.32×10^{-2}	-0.35×10^{-3}	0.58×10^{-4}	-0.49×10^{-4}	-0.22×10^{-3}
	-2	-0.10×10^{-2}	-0.19×10^{-3}	-0.65×10^{-4}	0.24×10^{-3}	0.14×10^{-3}
	-1	-0.52×10^{-2}	0.10×10^{-3}	0.42×10^{-4}	0.13×10^{-6}	-0.79×10^{-4}
	0	0.62×10^{-3}	-0.16×10^{-4}	0.41×10^{-6}	-0.94×10^{-5}	-0.19×10^{-4}
	1	0.27×10^{-2}	0.69×10^{-4}	0.28×10^{-3}	0.18×10^{-4}	0.19×10^{-3}
	2	-0.19×10^{-2}	-0.17×10^{-3}	0.25×10^{-3}	0.23×10^{-3}	0.23×10^{-3}
	3	-0.26×10^{-2}	0.14×10^{-3}	-0.11×10^{-3}	0.13×10^{-3}	0.28×10^{-3}
	4	-0.15×10^{-2}	-0.15×10^{-3}	0.21×10^{-3}	-0.47×10^{-4}	-0.23×10^{-4}
	5	0.31×10^{-1}	-0.56×10^{-3}	-0.67×10^{-3}	0.19×10^{-3}	0.16×10^{-3}
	6	0.60×10^{-3}	-0.24×10^{-3}	-0.16×10^{-3}	0.14×10^{-3}	0.47×10^{-4}