Supporting Information (SI)

Base and Anion Regulated Synthesis of Dysprosium Compounds

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Experimental

General information

All chemicals and solvents were obtained from commercial sources without further purification. All reactions were carried out under aerobic conditions. The elemental analyses (C, H, and N) were carried out using an Elementar Vario EL analyzer. Fourier transform IR spectra (4000 to 400 cm^{-1}) were measured on a Perkin-Elmer Spectrum GX spectrometer with samples prepared as KBr discs. Powder X-ray diffraction was carried out on a STOE STADI-P diffractometer, using Cu-Kα radiation with λ = 1.5406 Å.

Physical measurements

Variable-temperature dc magnetic susceptibility measurements and ac magnetic susceptibility measurements were conducted on microcrystalline samples, suspended in eicosane to prevent torquing, using a SQUID-based sample magnetometer, Quantum Design model MPMS3. Magnetic susceptibility data were collected under a 0.1 T applied magnetic field in temperature range 2-300 K. Magnetization isotherms were collected at 1.8, 2.5, 5 and 10 K between 0 and 70 kOe. Alternating current (ac) susceptibility measurements were carried out under an oscillating ac field of 2 Oe and ac frequencies ranging from 1 to 1000 Hz. Data were corrected for diamagnetism using Pascal constants and a sample holder correction.

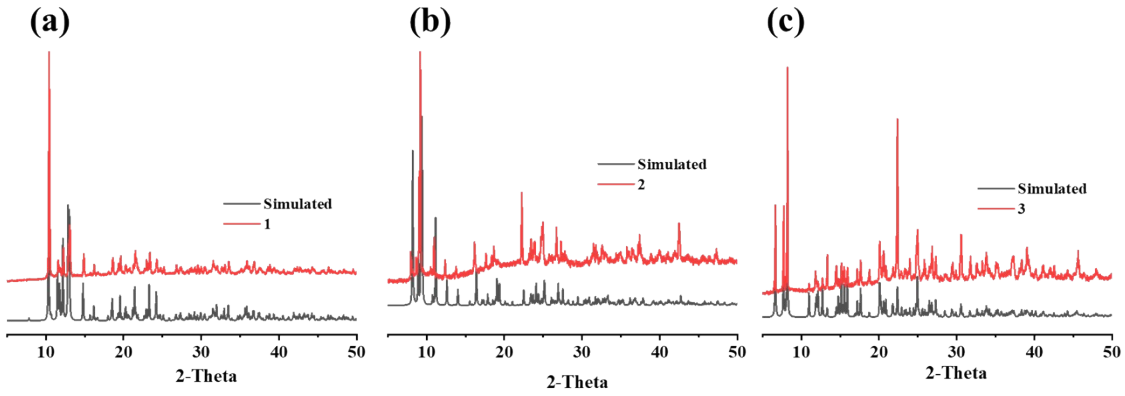

Fig.S1. Powder X-ray diffraction data for **1-3** (**a-c**).

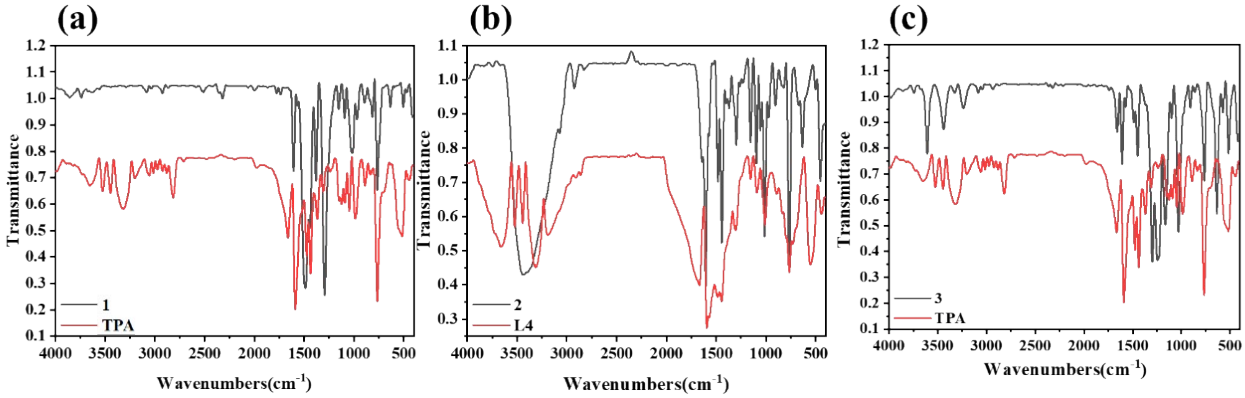

Fig.S2. IR spectroscopy of complexes **1-3** (**a-c**).

Table S1. The CShM values calculated by SHAPE for compounds **1**.

			1
Label	Shape	Symmetry	Distortion
DP-10	Decagon	D_{10h}	36.985
EPY-10	Enneagonal pyramid	C_{9v}	24.988
OBPY-10	Octagonal bipyramid	D_{8h}	17.369
PPR-10	Pentagonal prism	D_{5h}	8.263
PAPR-10	Pentagonal antiprism	D_{5d}	13.888
JBCCU-10	Bicapped cube J15	D_{4h}	13.804
JBCSAPR-10	Bicapped square antiprism J17	D_{4d}	6.118
JMBIC-10	Metabidiminished icosahedron J62	C_{2v}	10.246
JATDI-10	Augmented tridiminished icosahedron J64	C_{3v}	17.359
JSPC-10	Sphenocorona J87	$\boldsymbol{C_{2v}}$	**2.808**
SDD-10	Staggered Dodecahedron	D_2	7.222
TD-10	Tetradecahedron	C_{2v}	7.251
HD-10	Hexadecahedron	D_{4h}	11.553

Table S2. The CShM values calculated by SHAPE 2.1 for compounds **2** and **3**.

			2	**3**
Label	Shape	Symmetry	Distortion	
OP-8	Octagon	D_{8h}	30.78	30.55
HPY-8	Heptagonal pyramid	C_{7v}	24.21	22.91
HBPY-8	Hexagonal bipyramid	D_{6h}	16.51	16.02
CU-8	Cube	O_h	10.35	10.90
SAPR-8	Square antiprism	$\boldsymbol{D_{4d}}$	2.12	**1.06**
TDD-8	Triangular dodecahedron	$\boldsymbol{D_{2d}}$	**1.08**	1.74
JGBF-8	Johnson gyrobifastigium J26	D_{2d}	14.76	14.94
JETBPY-8	Johnson elongated triangular bipyramid J14	D_{3h}	28.50	27.54
JBTPR-8	Biaugmented trigonal prism J50	C_{2v}	3.24	2.59
BTPR-8	Biaugmented trigonal prism	C_{2v}	2.43	2.12
JSD-8	Snub diphenoid J84	D_{2d}	3.78	4.39
TT-8	Triakis tetrahedron	T_d	11.05	11.73
ETBPY-8	Elongated trigonal bipyramid	D_{3h}	24.59	23.42

Table S3. Selected bond distances (Å) for compounds **1**–**3.**

1		**2**		**3**	
Dy1–O1	2.473(3)	Dy1–O1	2.217(5)	Dy1–O1	2.249(2)
Dy1–O2	2.449(3)	Dy1–O1$^{\#}$	2.254(5)	Dy1–O1$^{\#}$	2.256(3)
Dy1–O3	2.460(2)	Dy1–O2	2.470(6)	Dy1–O2	2.392(2)
Dy1–O4	2.490(2)	**Dy1–Cl1**	**2.666(2)**	**Dy1–O3**	**2.407(2)**
Dy1–O5	2.440(2)	Dy1–N1	2.617(6)	Dy1–N1	2.557(3)
Dy1–O6	2.450(3)	Dy1–N2	2.567(4)	Dy1–N2	2.627(3)
Dy1–N1	2.557(3)	Dy1–N3	2.581(6)	Dy1–N3	2.528(3)
Dy1–N2	2.654(3)	Dy1–N4	2.613(6)	Dy1–N4	2.576(3)
Dy1–N3	2.604(3)				
Dy1–N4	2.553(3)				

Table S4. Selected bond angles (°) for compounds **1**–**3**.

1		**2**		**3**	
O6–Dy1–O3	121.49(9)	O1–Dy1–O1$^{\#}$	70.28(13)	O1–Dy1–O1$^{\#}$	69.30(11)
O6–Dy1–O1	118.10(9)	O1$^{\#}$–Dy1–O2	79.38(11)	O1$^{\#}$–Dy1–O3	82.85(9)
O6–Dy1–O4	118.83(9)	O1–Dy1–O2	147.74(12)	O1–Dy1–O3	148.53(9)
O5–Dy1–O6	52.34(9)	O1–Dy1–N4	78.76(11)	O1$^{\#}$–Dy1–O2	82.50(9)
O5–Dy1–O3	72.65(9)	O1$^{\#}$–Dy1–N4	130.25(11)	O1–Dy1–O2	110.55(9)
O5–Dy1–O2	73.67(10)	O1–Dy1–N3	87.98(13)	O3–Dy1–O2	78.79(9)
O5–Dy1–O1	122.08(9)	O1$^{\#}$–Dy1–N3	76.48(12)	O1$^{\#}$–Dy1–N1	130.57(9)
O5–Dy1–O4	74.62(8)	O1$^{\#}$–Dy1–N1	137.61(12)	O1–Dy1–N1	76.37(9)
		O1–Dy1–N1	77.65(12)	O1–Dy1–N3	85.66(10)
		O1–Dy1–N2	138.65(10)	O1$^{\#}$–Dy1–N2	149.89(9)
		O1$^{\#}$–Dy1–N2	150.57(11)	O1–Dy1–N2	140.30(9)

	Dy1–O1–Dy1#	109.72(13)	Dy1–O1–Dy1#	110.70(11)

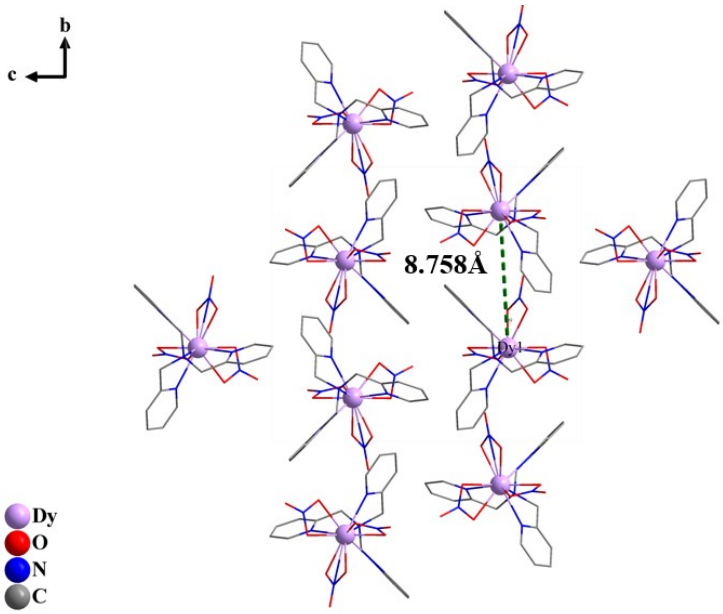

Fig S3. Packing of complex **1**. Dash lines are the shortest distance of intramolecular Dy-Dy distances

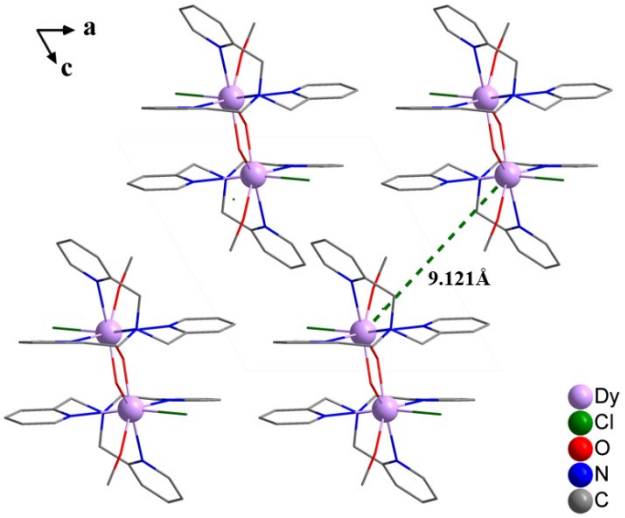

Fig S4. Packing of complex **2**. Dash lines are the shortest distance of intramolecular Dy-Dy distances

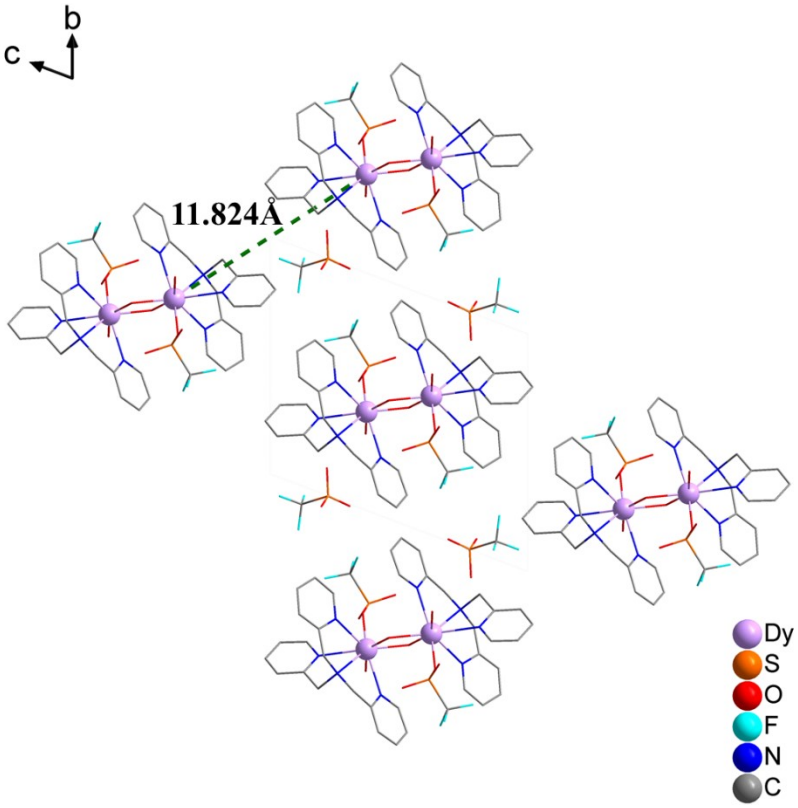

Fig S5. Packing of complex **3**. Dash lines are the shortest distance of intramolecular Dy-Dy distances

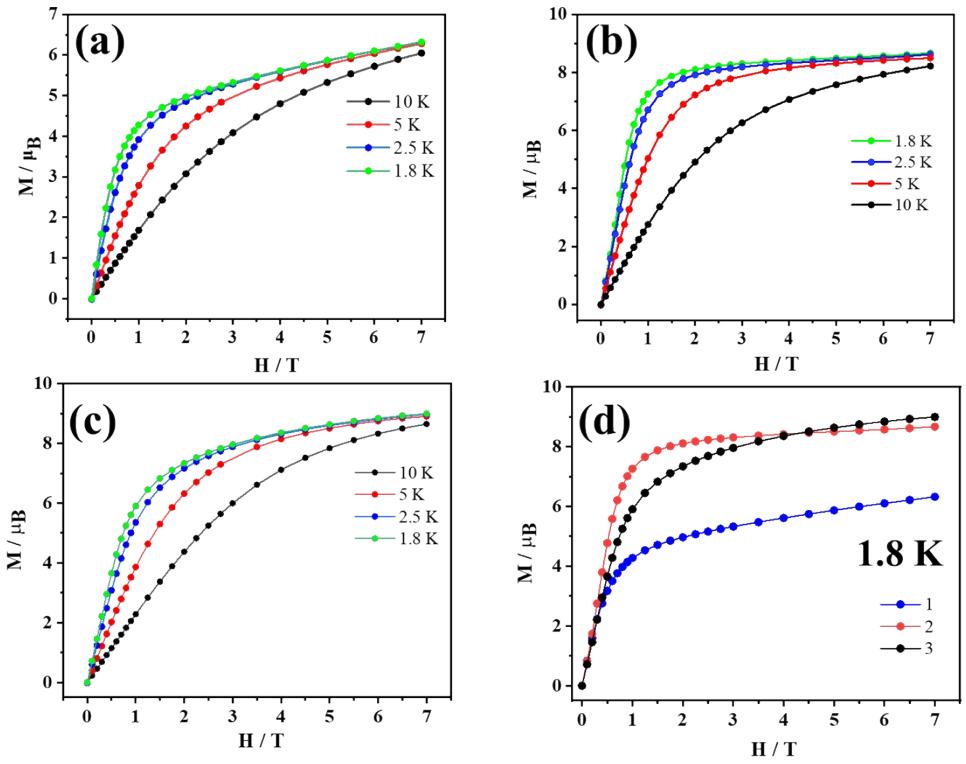

Fig S6. Field dependence of the magnetization for **1** (a), **2** (b), **3** (c) at corresponding temperatures and at 1.8 K for **1-3** (d).

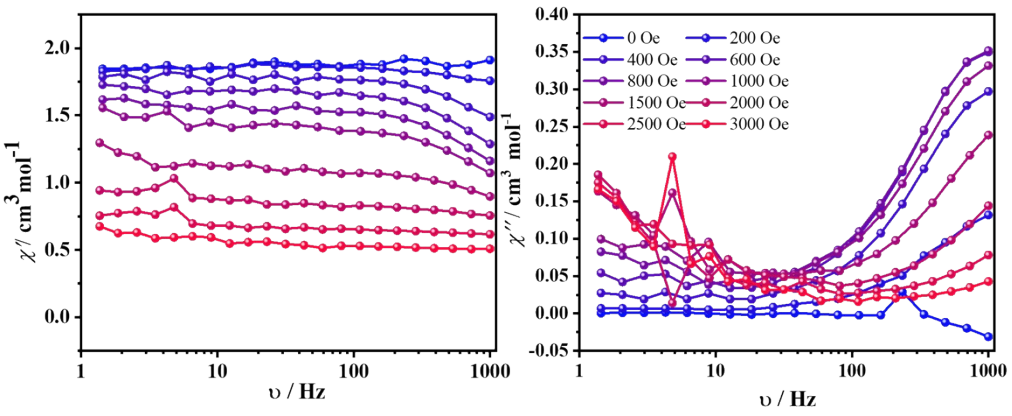

Fig S7. Plots of χ' (left) and χ'' (right) vs frequency under different dc field for **1** at 2 K.

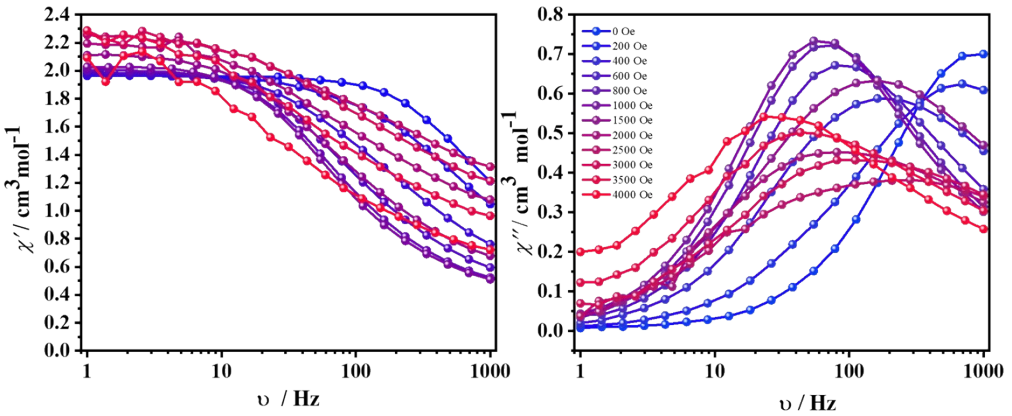

Fig S8. Plots of χ' (left) and χ'' (right) vs frequency under different dc field for **2** at 2 K.

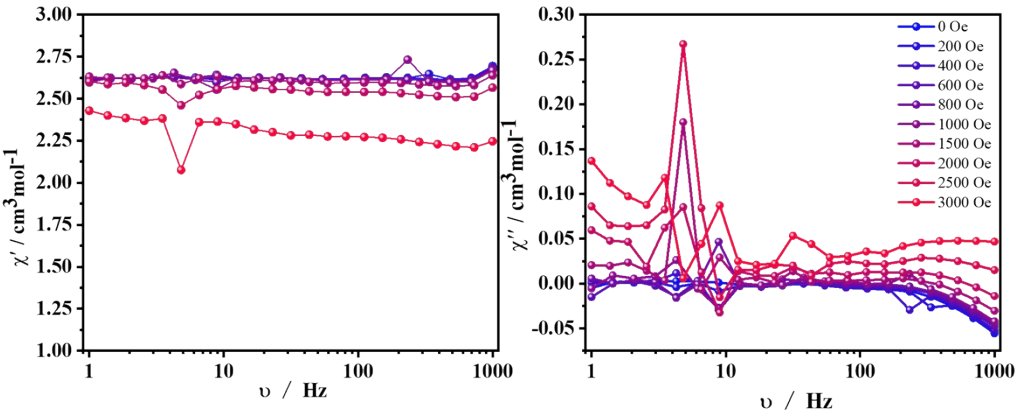

Fig S9. Plots of χ' (left) and χ'' (right) vs frequency under different dc field for **3** at 2 K.

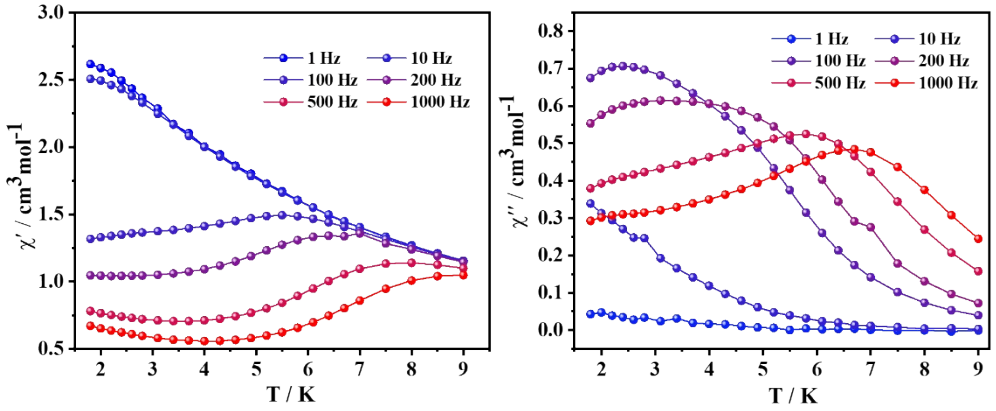

Fig S10. Plots of χ' (left) and χ'' (right) vs temperature under different frequency for **2**.

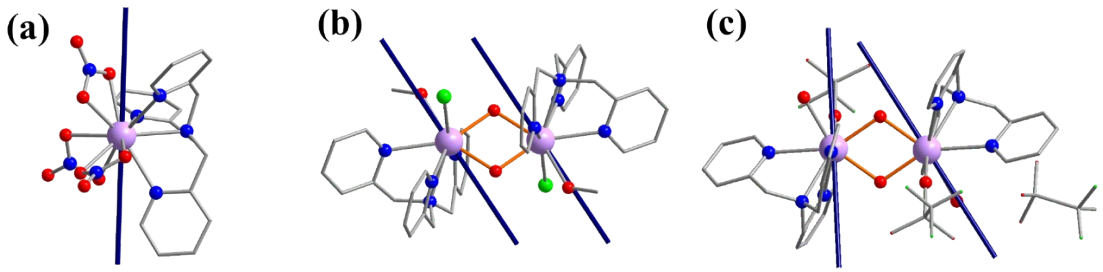

Fig S11. The magnetic axes for complexes **1** (a), **2** (b) and **3** (c).

Table S5. The parameters fitted by Cfit2 at 1.8-7 K (generalized Debye model）

T	τ	χ_S	χ_T	α
1.800195	2.35E-03	5.39E+02	2.51E+03	2.20E-01
2.000584	2.17E-03	5.13E+02	2.49E+03	2.15E-01
2.200195	2.00E-03	4.93E+02	2.44E+03	2.09E-01
2.400016	1.86E-03	4.75E+02	2.39E+03	2.05E-01
2.600095	1.72E-03	4.57E+02	2.34E+03	2.02E-01
2.79997	1.59E-03	4.40E+02	2.27E+03	1.99E-01
3.100121	1.41E-03	4.19E+02	2.19E+03	1.94E-01
3.400218	1.24E-03	3.97E+02	2.09E+03	1.89E-01
3.700054	1.09E-03	3.82E+02	2.01E+03	1.82E-01
4.000182	9.54E-04	3.70E+02	1.92E+03	1.71E-01
4.300102	8.29E-04	3.59E+02	1.84E+03	1.62E-01
4.60021	7.19E-04	3.57E+02	1.77E+03	1.48E-01
4.89989	6.10E-04	3.51E+02	1.70E+03	1.34E-01
5.200179	5.17E-04	3.48E+02	1.64E+03	1.20E-01
5.499902	4.35E-04	3.46E+02	1.57E+03	1.07E-01
5.799762	3.62E-04	3.44E+02	1.51E+03	9.07E-02
6.100094	3.02E-04	3.40E+02	1.46E+03	8.28E-02
6.399963	2.50E-04	3.33E+02	1.41E+03	7.80E-02

6.699955	2.06E-04	3.26E+02	1.36E+03	7.50E-02
6.999777	1.76E-04	3.33E+02	1.32E+03	6.68E-02

Table S6. The input file of complex **1** for Magellan software.

Atom Type	X	Y	Z	Valence
Dy	4.07509	5.13094	4.05867	3
O	4.61206	7.27441	3.00105	-2/3
O	2.75539	7.18371	4.09352	-2/3
O	1.75458	4.50249	4.58338	-2/3
O	2.78468	5.15486	1.97707	-2/3
O	3.49652	3.22228	2.59641	-2/3
O	2.92279	5.13756	6.26616	-2/3
N	4.44116	2.89872	5.25157	0
N	6.46247	4.65502	4.83139	0
N	5.12631	6.81037	5.82428	0
N	5.85651	4.89764	2.17315	0
O	0.81551	4.71564	6.5251	-2/3
N	1.80138	4.78212	5.81369	0
N	3.58876	7.88346	3.42977	0
N	2.84108	3.90939	1.75297	0
O	2.30011	3.40849	0.7857	-2/3
O	3.402	9.06575	3.21626	-2/3
C	5.48659	2.78426	6.08305	0
C	3.56862	1.87422	5.20443	0
C	7.17899	5.95208	4.95164	0
C	6.43219	3.95151	6.12849	0
C	7.18192	3.81312	3.84995	0
C	6.46362	6.88468	5.85862	0
C	4.4482	7.62173	6.65798	0
C	5.67412	5.32784	0.91381	0
C	7.03808	4.35463	2.46984	0
C	5.65834	1.67567	6.87832	0
C	3.68338	0.7551	5.97647	0
C	4.74195	0.65884	6.82879	0
C	7.13194	7.76613	6.6819	0
C	6.41372	8.57689	7.52055	0
C	5.05597	8.48965	7.52738	0
C	7.8425	4.68104	0.26304	0
C	6.64183	5.21503	-0.06661	0
C	8.0599	4.25686	1.54066	0

Table S7. The input file of complex **2** for Magellan software.

Atom Type	X	Y	Z	Valence
Dy	7.2742	4.60332	1.61885	3
Cl	9.86006	5.21608	1.83258	-1
O	6.83791	4.2332	-0.52317	-1
O	7.15793	6.56915	0.52317	-1
O	7.24293	6.18735	3.51427	0
N	5.5494	2.6482	1.78195	0
N	4.80591	5.29938	1.91001	0
N	8.31854	2.23379	1.23794	0
N	7.43341	3.27243	3.80911	0
Dy	6.72164	6.19903	-1.61885	3
C	6.02771	1.45066	1.05329	0
C	4.2736	3.07266	1.15157	0
C	5.31044	2.3172	3.19461	0
C	3.83003	4.43075	1.62212	0
C	4.44175	6.5681	2.19294	0
C	7.48193	1.17501	1.20021	0
C	9.62734	1.97428	1.24091	0
C	6.55773	2.20197	3.95305	0
C	8.61215	3.31039	4.54373	0
Cl	4.13578	5.58627	-1.83258	-1
O	6.75291	4.615	-3.51427	0
N	8.44645	8.15415	-1.78195	0
N	9.18993	5.50297	-1.91001	0
N	5.67731	8.56856	-1.23794	0
N	6.56243	7.52992	-3.80911	0
C	2.48386	4.78741	1.68566	0
C	3.12237	6.98772	2.2396	0
C	7.93961	-0.13291	1.19723	0
C	10.146	0.69449	1.21113	0
C	6.86163	1.17048	4.83261	0
C	8.91548	2.27881	5.42428	0
C	8.04092	1.20836	5.56823	0
C	2.13927	6.07362	1.99241	0
C	9.27869	-0.3556	1.19922	0
C	6.69025	6.21572	4.81276	0
C	7.96813	9.35169	-1.05329	0
C	9.72224	7.72969	-1.15157	0
C	8.6854	8.48515	-3.19461	0
C	10.16581	6.3716	-1.62212	0
C	9.55409	4.23425	-2.19294	0
C	6.51392	9.62734	-1.20021	0
C	4.36851	8.82806	-1.24091	0

C	7.43811	8.60038	-3.95305	0
C	5.3837	7.49196	-4.54373	0
C	6.05624	10.93526	-1.19723	0
C	4.71715	11.15795	-1.19922	0
C	3.84984	10.10786	-1.21113	0
C	11.51198	6.01494	-1.68566	0
C	11.85657	4.72873	-1.99241	0
C	10.87348	3.81463	-2.2396	0
C	7.13422	9.63187	-4.83261	0
C	5.95492	9.59399	-5.56823	0
C	5.08036	8.52354	-5.42428	0
C	7.30559	4.58663	-4.81276	0

Table S8. Table S7. The input file of complex **3** for Magellan software.

Atom Type	X	Y	Z	Valence
Dy	5.80471	8.23367	8.31402	+3
Dy	7.16549	9.04438	4.96235	+3
O	7.64062	8.8257	7.1576	-1
O	5.32927	8.45255	6.11934	0
O	3.69237	7.1119	8.35518	-1/3
O	4.29076	10.09534	8.50521	-1/3
O	1.88263	9.82362	8.70702	-1/3
O	2.80756	11.03593	6.83497	-1/3
O	9.27722	10.16644	4.92185	-1/3
O	8.67911	7.18236	4.77113	-1/3
O	11.08719	7.45461	4.56939	-1
O	10.16219	6.24209	6.44213	0
N	7.48251	6.98986	9.82095	0
N	7.04408	9.80067	9.90991	0
N	6.33352	5.87533	7.57449	0
N	5	7.8933	10.79017	0
S	2.9615	10.59962	8.18922	0
C	2.90768	12.14816	9.15312	0
F	1.74177	12.7487	8.99114	0
C	8.42485	7.89285	10.5233	0
C	8.27104	6.06477	8.97919	0
C	6.70136	6.20168	10.80876	0
C	6.77337	11.11329	10.02011	0
C	7.93137	9.27997	10.76893	0
C	5.59634	5.20212	6.66635	0
C	7.40403	5.25134	8.06972	0
C	4.07305	8.62047	11.40356	0
C	5.72503	7.05673	11.54961	0
F	3.06073	11.90367	10.44099	0

C	7.33926	11.93003	10.97074	0
F	3.85661	12.97402	8.78004	0
C	5.90377	3.94294	6.23087	0
C	3.85576	8.58967	12.76711	0
C	8.48764	10.03872	11.78328	0
C	5.56596	6.97963	12.91713	0
C	7.75732	3.9663	7.70195	0
C	8.20026	11.36909	11.87888	0
C	6.99842	3.30487	6.76991	0
C	4.6261	7.7546	13.53053	0
N	5.4874	10.28812	3.45591	0
N	5.92593	7.4777	3.36677	0
N	6.6364	11.40267	5.70223	0
N	7.96991	9.38515	2.48672	0
S	10.00856	6.67843	5.08719	0
C	4.54536	9.38539	2.75335	0
C	4.69887	11.21365	4.2979	0
C	6.26892	11.07651	2.4681	0
C	6.19679	6.16547	3.25658	0
C	5.03898	7.99841	2.50781	0
C	7.37382	12.07657	6.61066	0
C	5.56634	12.02736	5.20712	0
C	8.8972	8.65827	1.8733	0
C	7.24527	10.22184	1.72743	0
C	5.63053	5.34771	2.30605	0
C	4.4823	7.23947	1.49326	0
C	7.40403	10.2987	0.35957	0
C	4.76936	5.90957	1.39766	0
C	8.34363	9.52394	-0.25386	0
C	7.06589	13.33518	7.04585	0
C	5.97123	13.97324	6.50698	0
C	5.21268	13.31214	5.57508	0
C	10.06235	5.13018	4.12369	0
F	11.22794	4.52985	4.28578	0
F	9.90908	5.37503	2.83605	0
F	9.11308	4.30435	4.49647	0
C	9.11424	8.68804	0.50952	0