Electronic Supplementary Information

Tuning the Antiferromagnetic Interaction of Lanthanide-Porphyrin Complexes with Varied Cyclododecane Ligands in Photo-Excitation State

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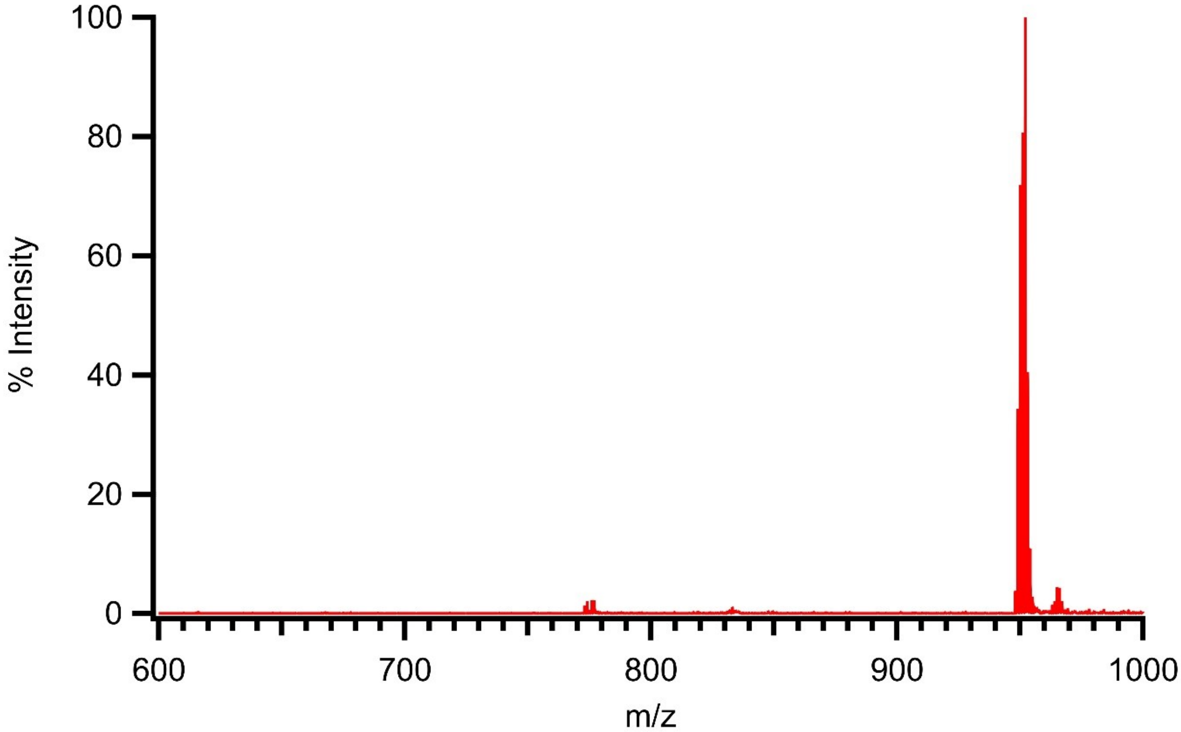

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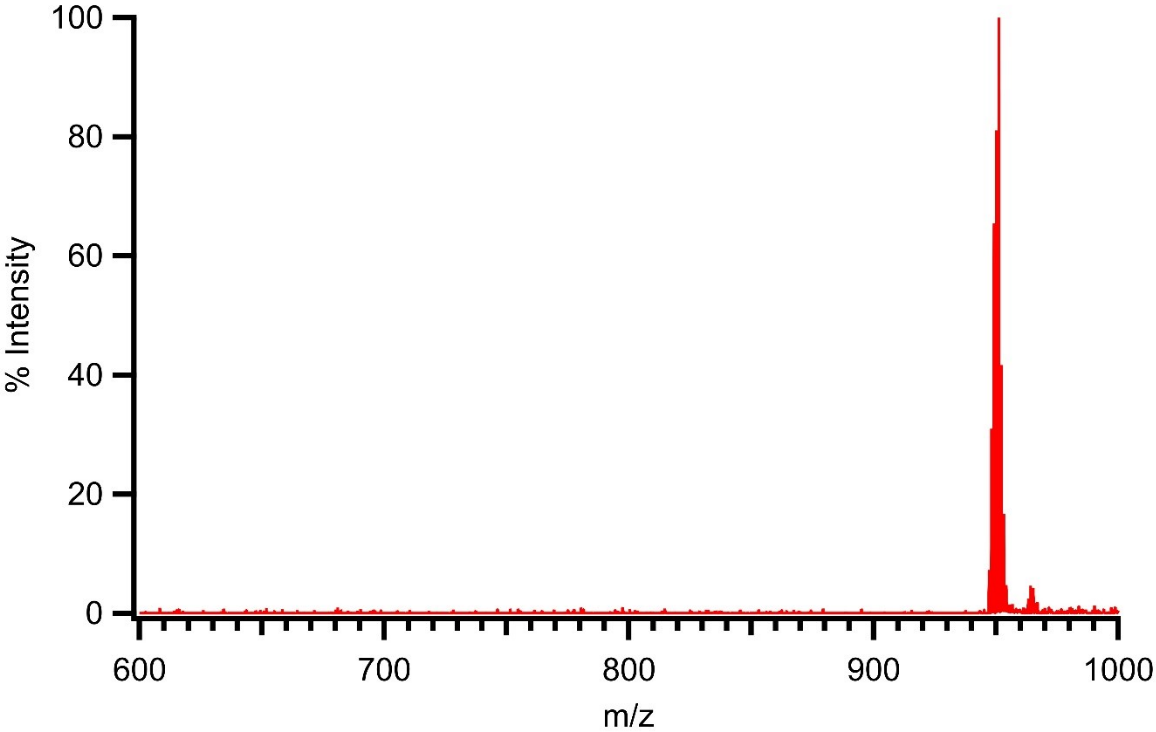

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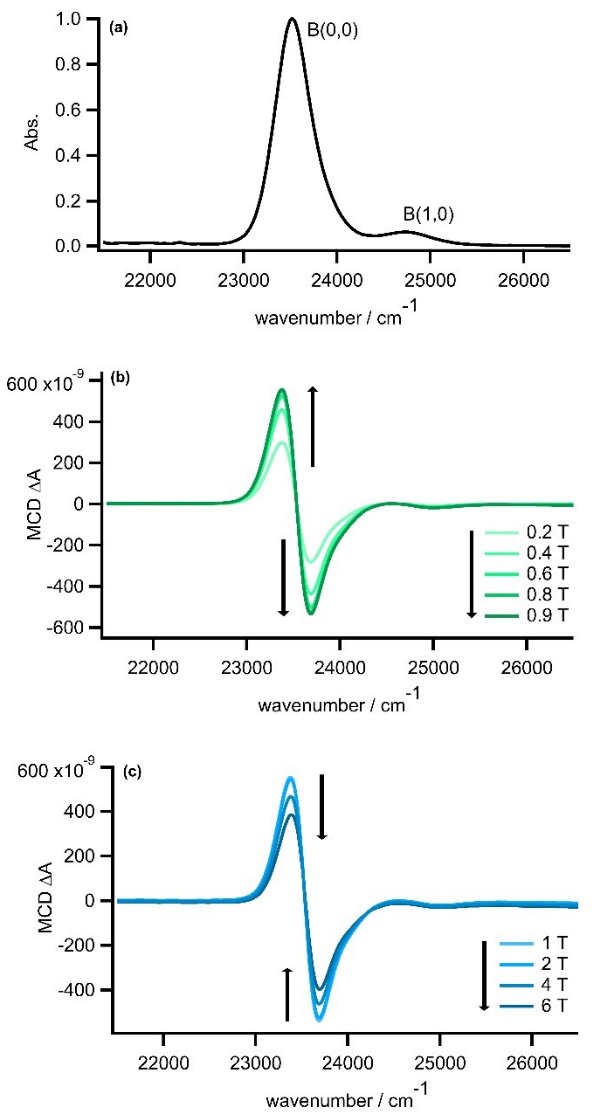

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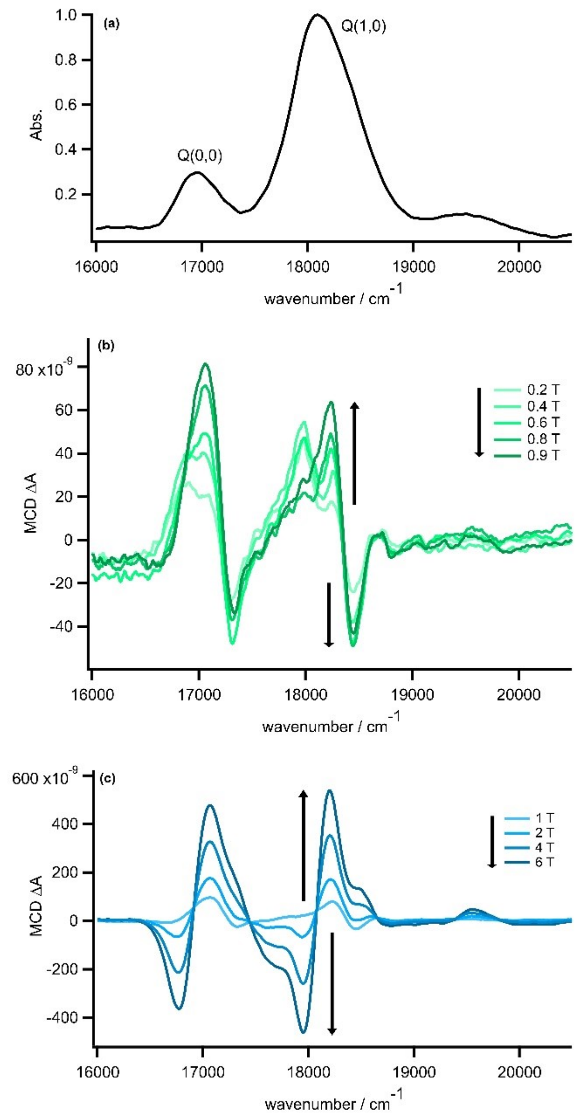

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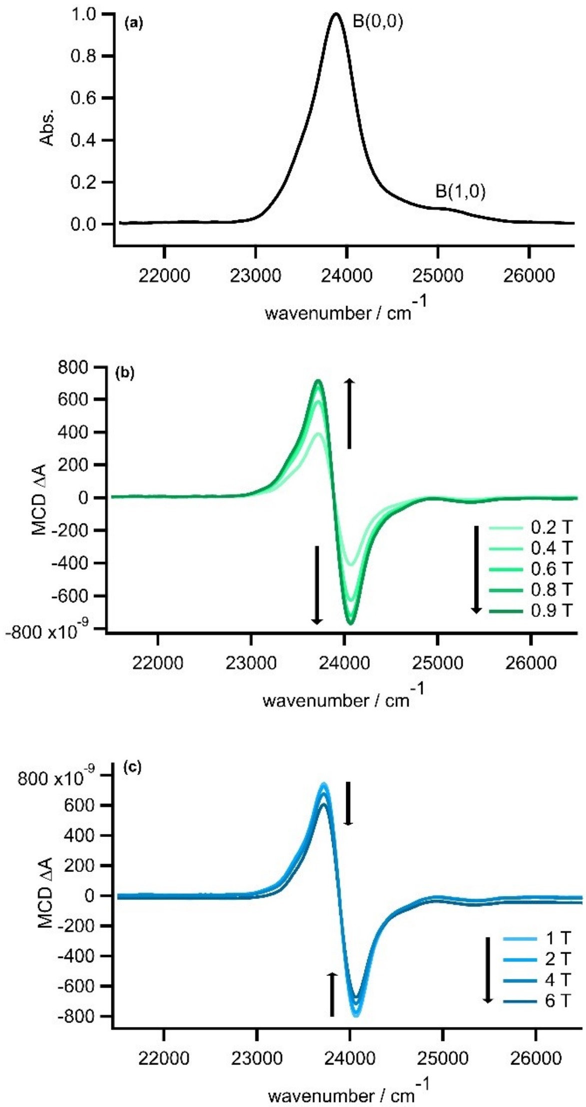

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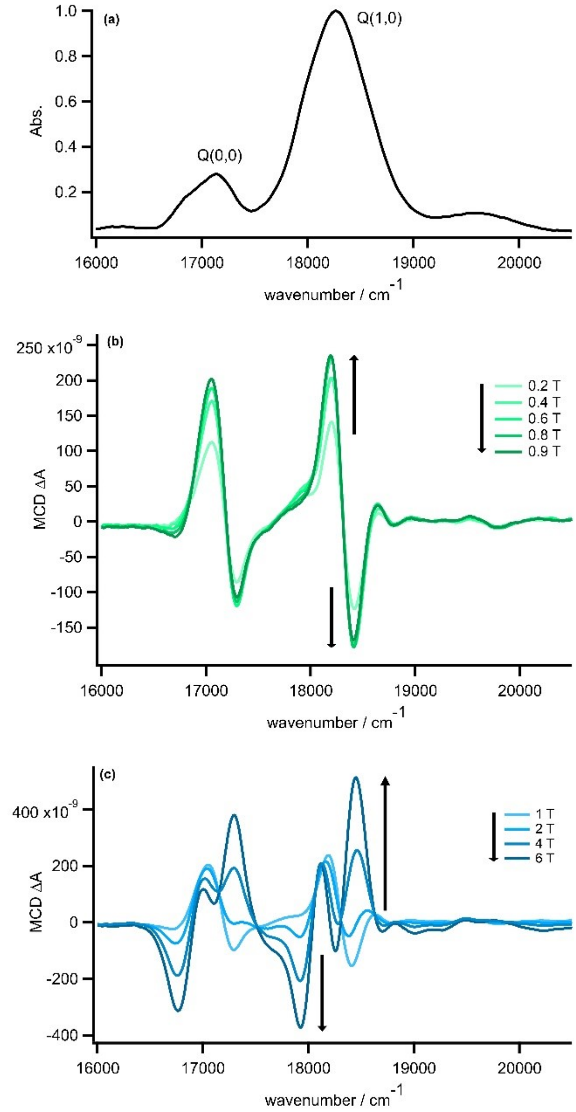

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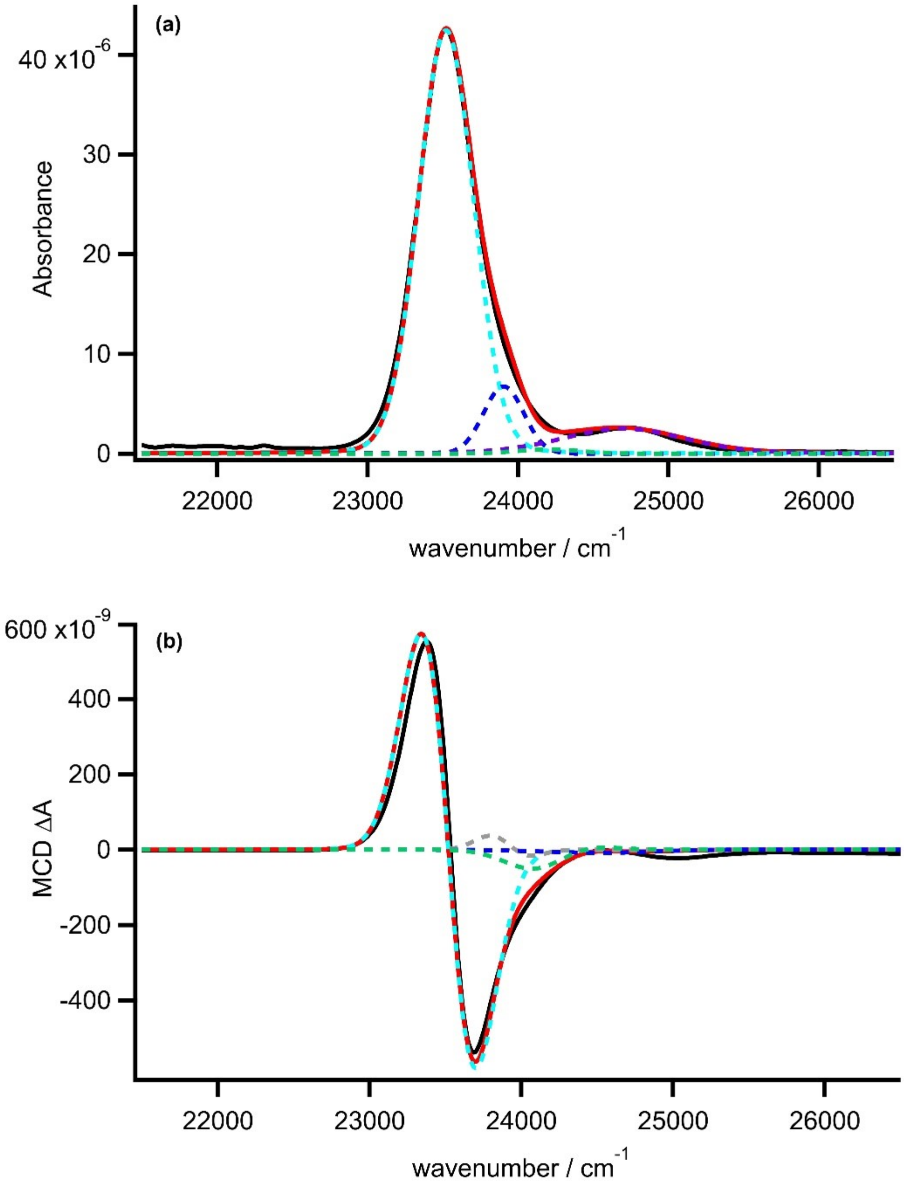

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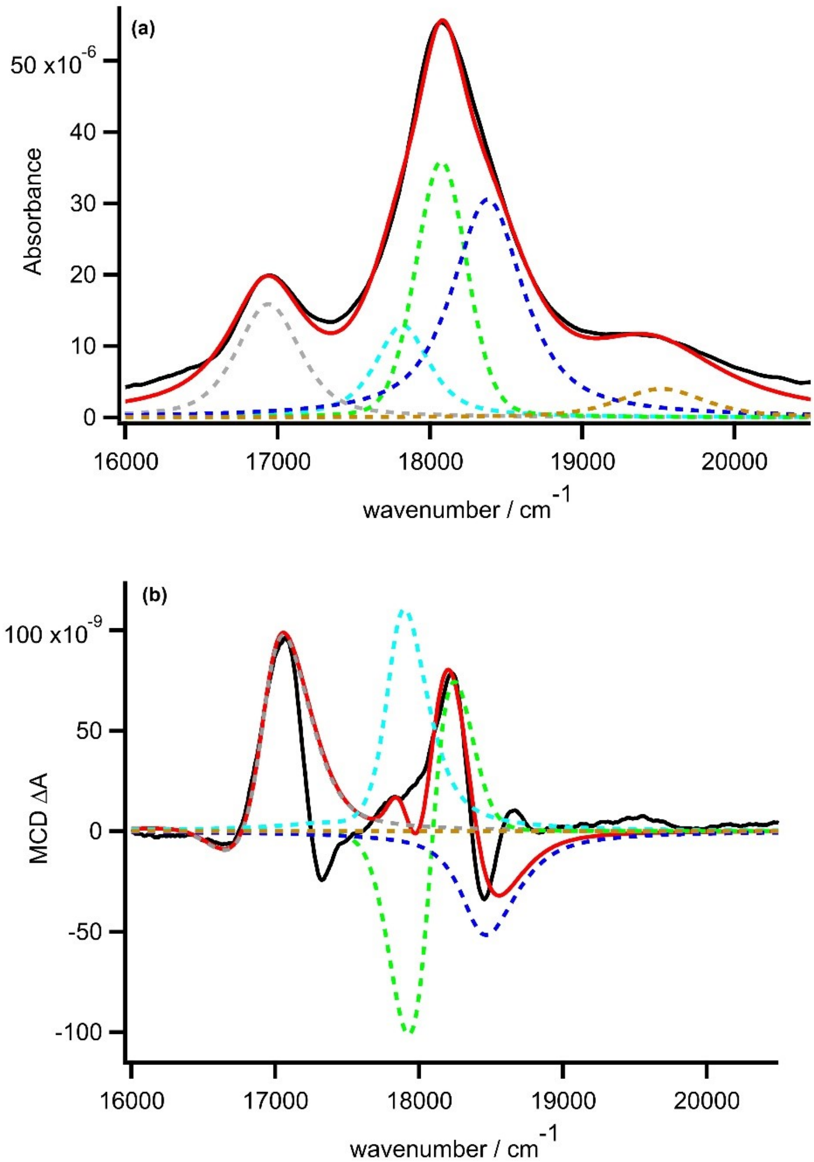

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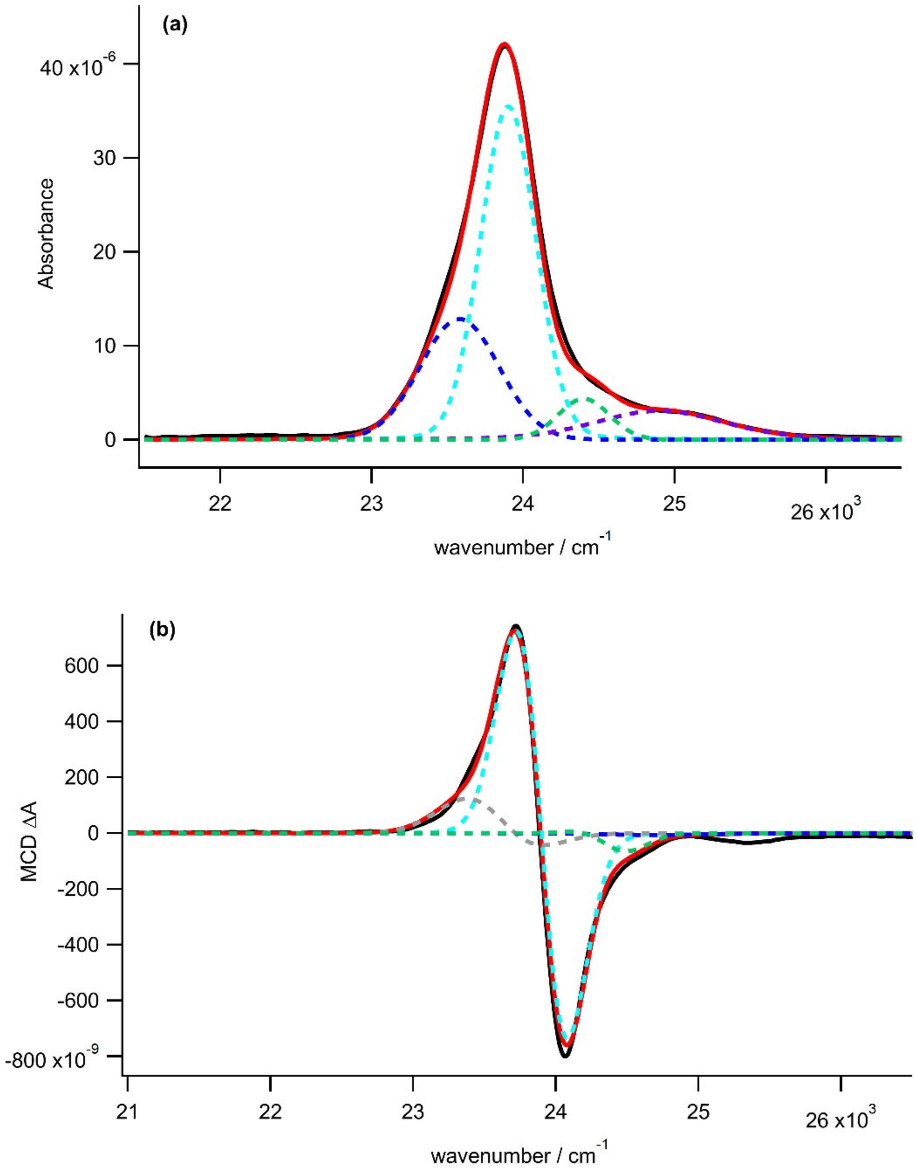

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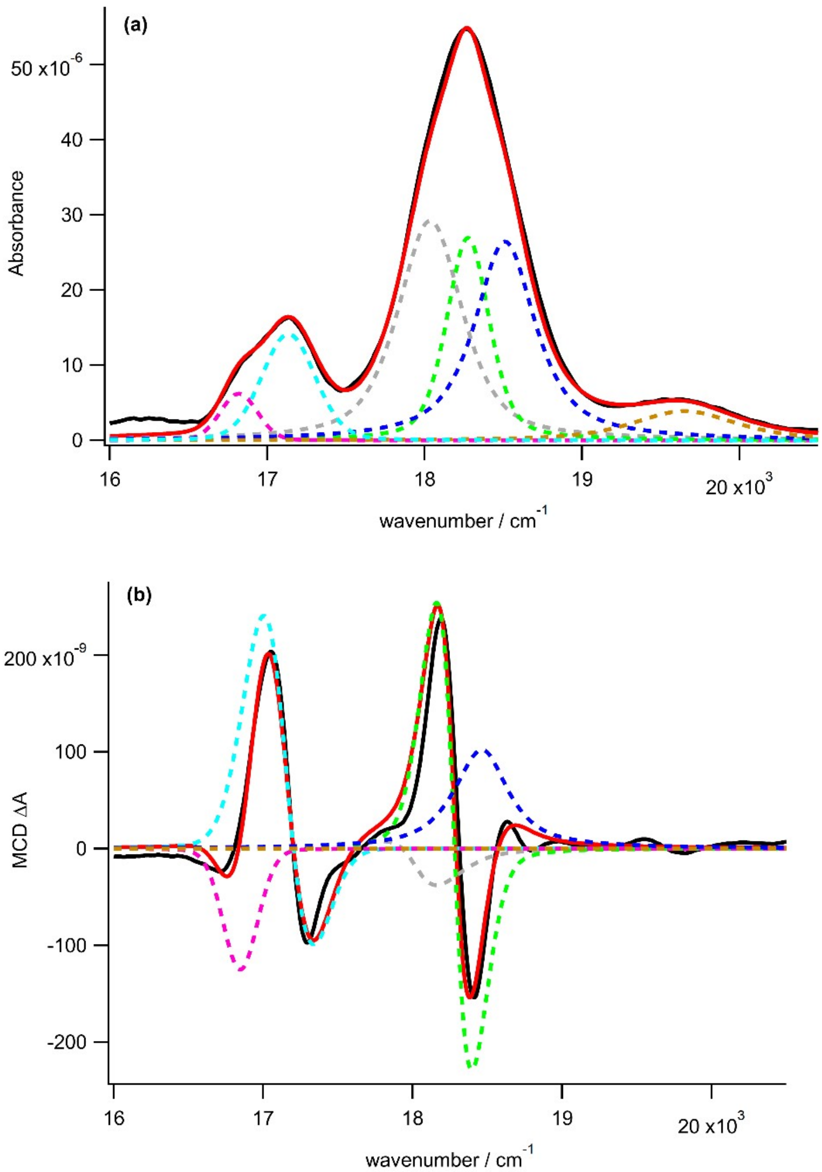

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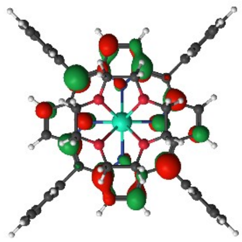
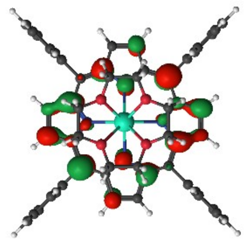
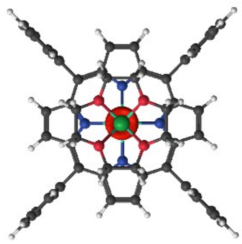
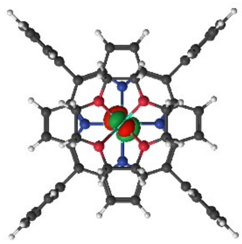
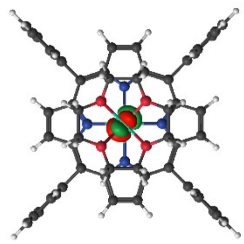
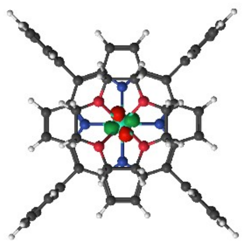
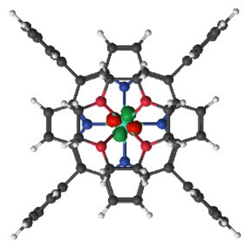
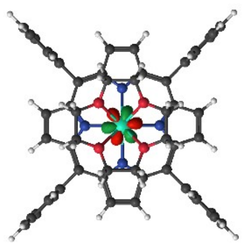
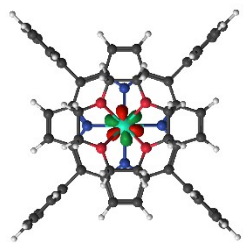
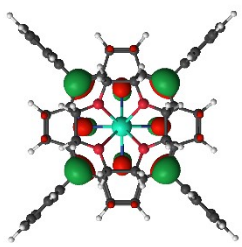
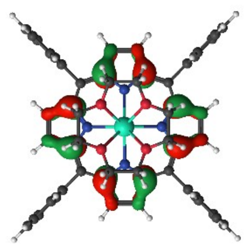
π* orbitals		
$4f_0$		
$4f_{1-}/4f_{1+}$		
$4f_{2-}/4f_{2+}$		
$4f_{3-}/4f_{3+}$		
π orbitals		

Figure S11. Selected molecular orbitals of $[Dy(TPP)(12C4)]^+$ generated from CAS(9,7) calculation.

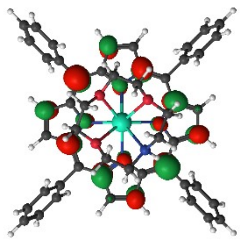
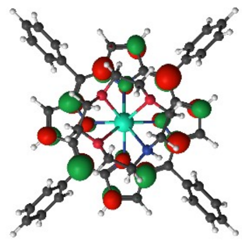
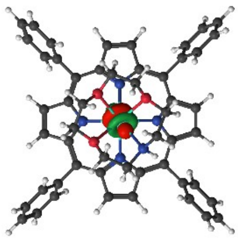
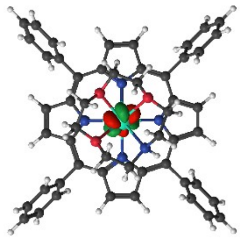
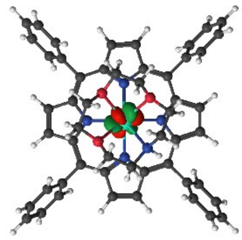
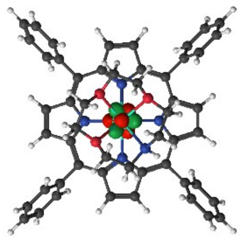
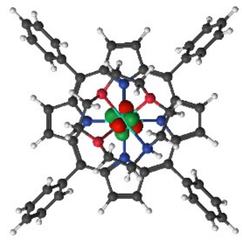
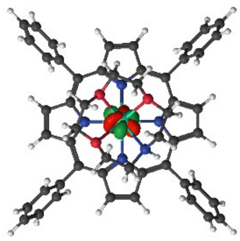
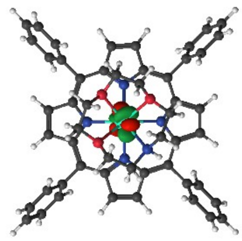
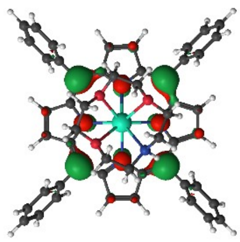
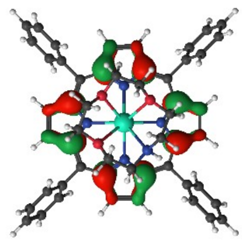
π* orbitals		
$4f_0$		
$4f_{1-}/4f_{1+}$		
$4f_{2-}/4f_{2+}$		
$4f_{3-}/4f_{3+}$		
π orbitals		

Figure S12. Selected molecular orbitals of $[Dy(TPP)(aza12C4)]^+$ generated from CAS(9,7) calculation

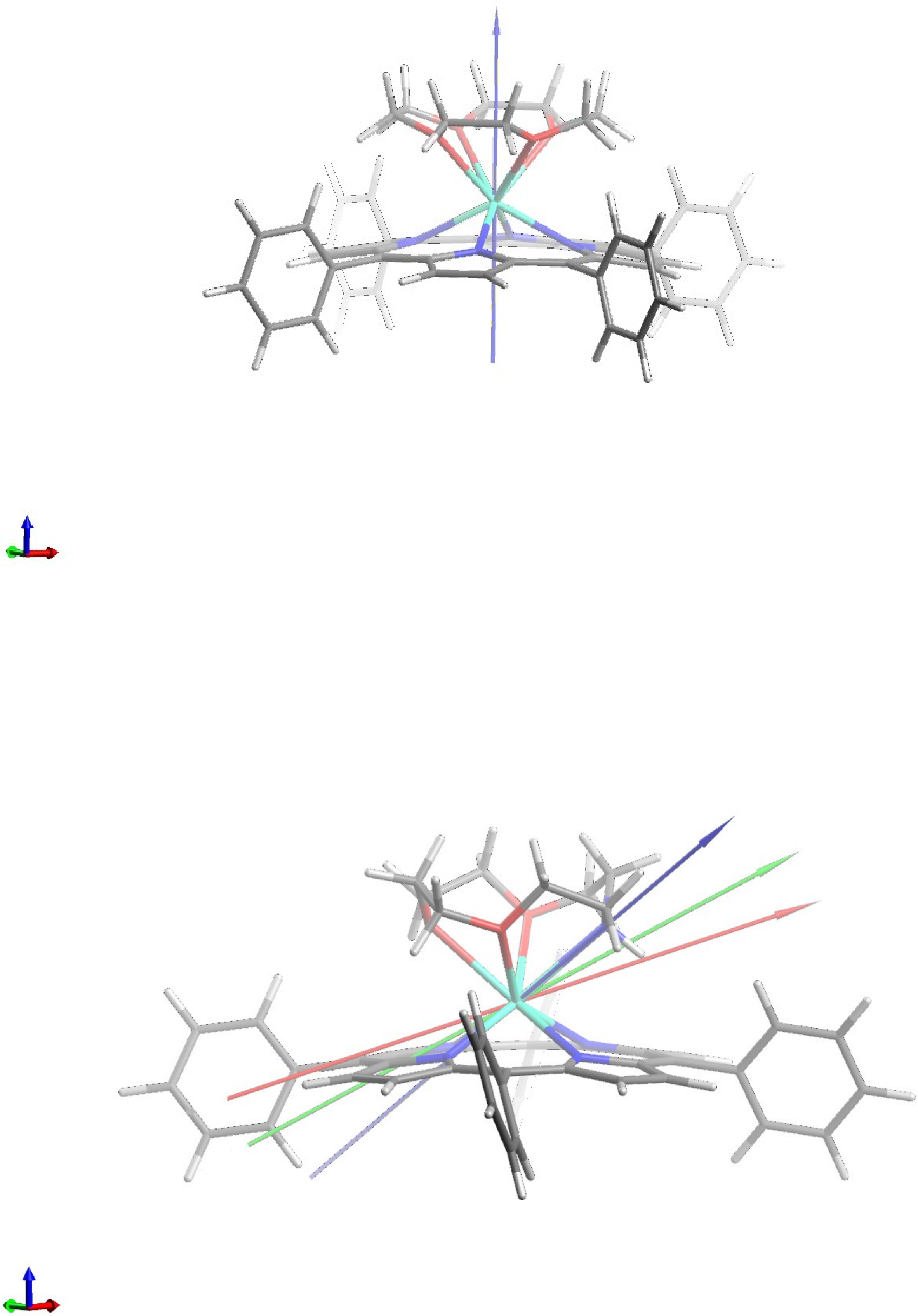


Figure S13. Main magnetic axes of the [Dy(TPP)(12C4)]$^+$ (top) and [Dy(TPP)(aza12C4)]$^+$ (bottom) extracted from CASSCF/RASSI/SINGLE_ANISO calculations.

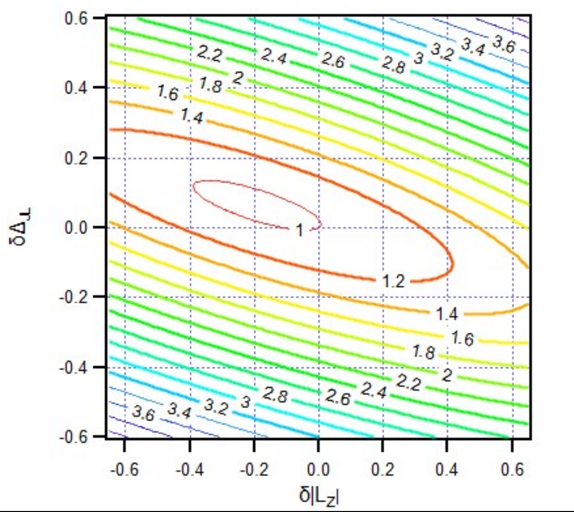
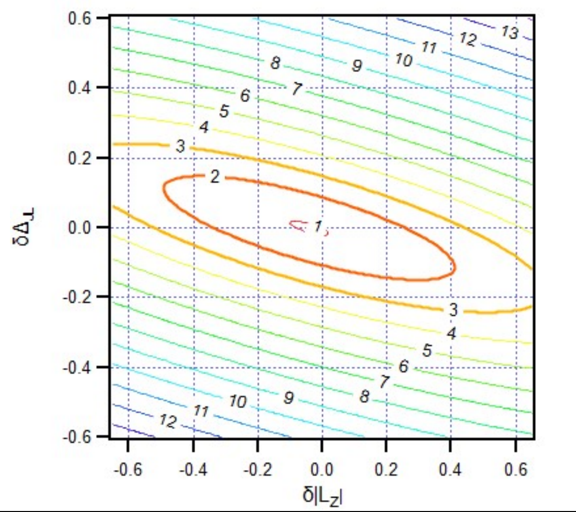
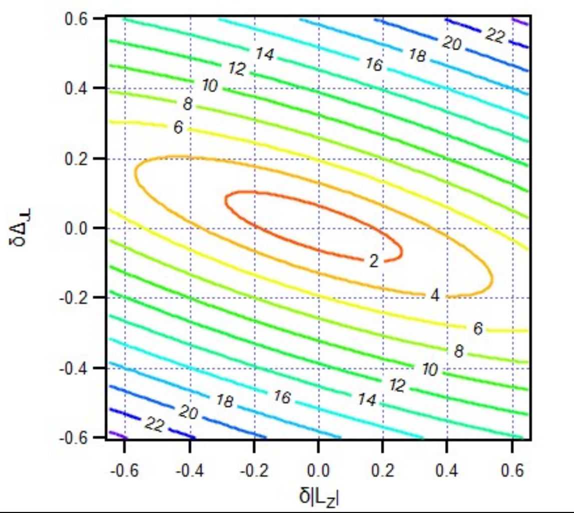
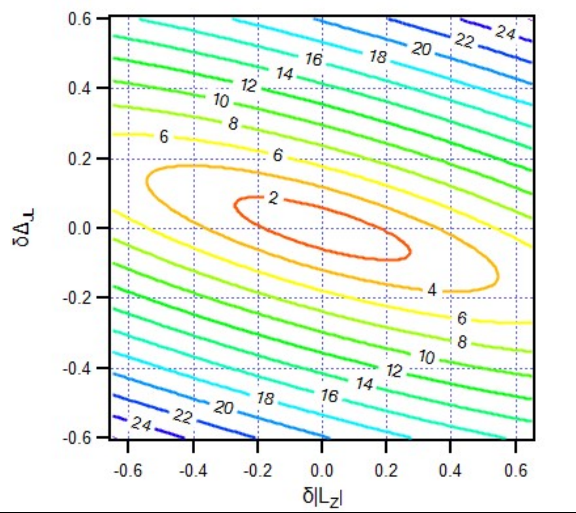
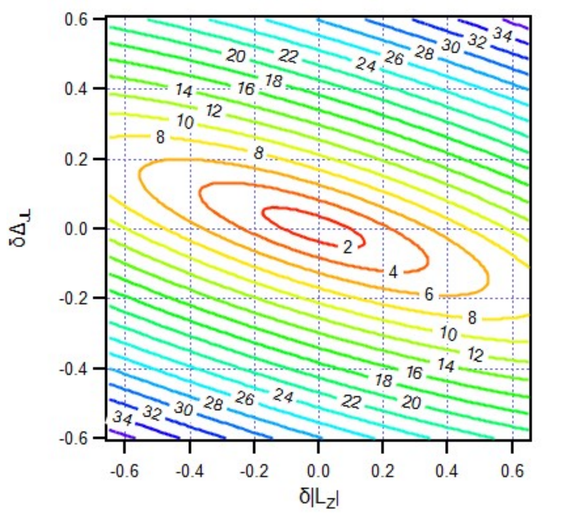
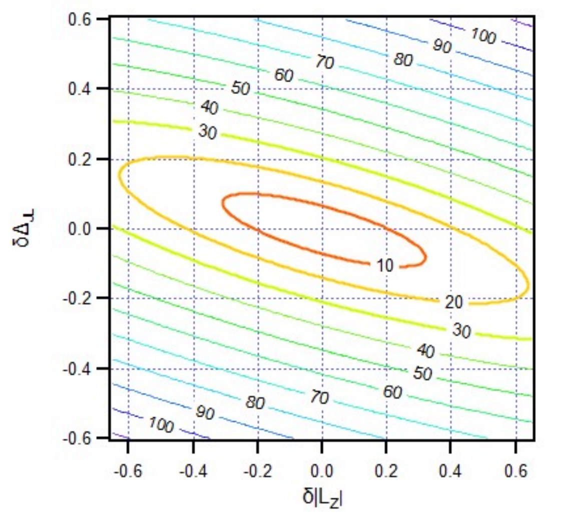
	Jz = 11/2	Jz = 13/2
B(0,0)		
Q(1,0)		
Q(0,0)		

Figure S14. Contour maps of the ratio RMS1/RMS0 for $[Dy(TPP)(12C4)]^{+}$, where RMS0 is the minimum RMS error obtained with the two parameters ($|L_z|$ and Δ_{JL}) determined by means of least-square procedure, and RMS1 is the RMS error obtained varying two parameters of the two by the values indicated in the vertical and horizontal axes.

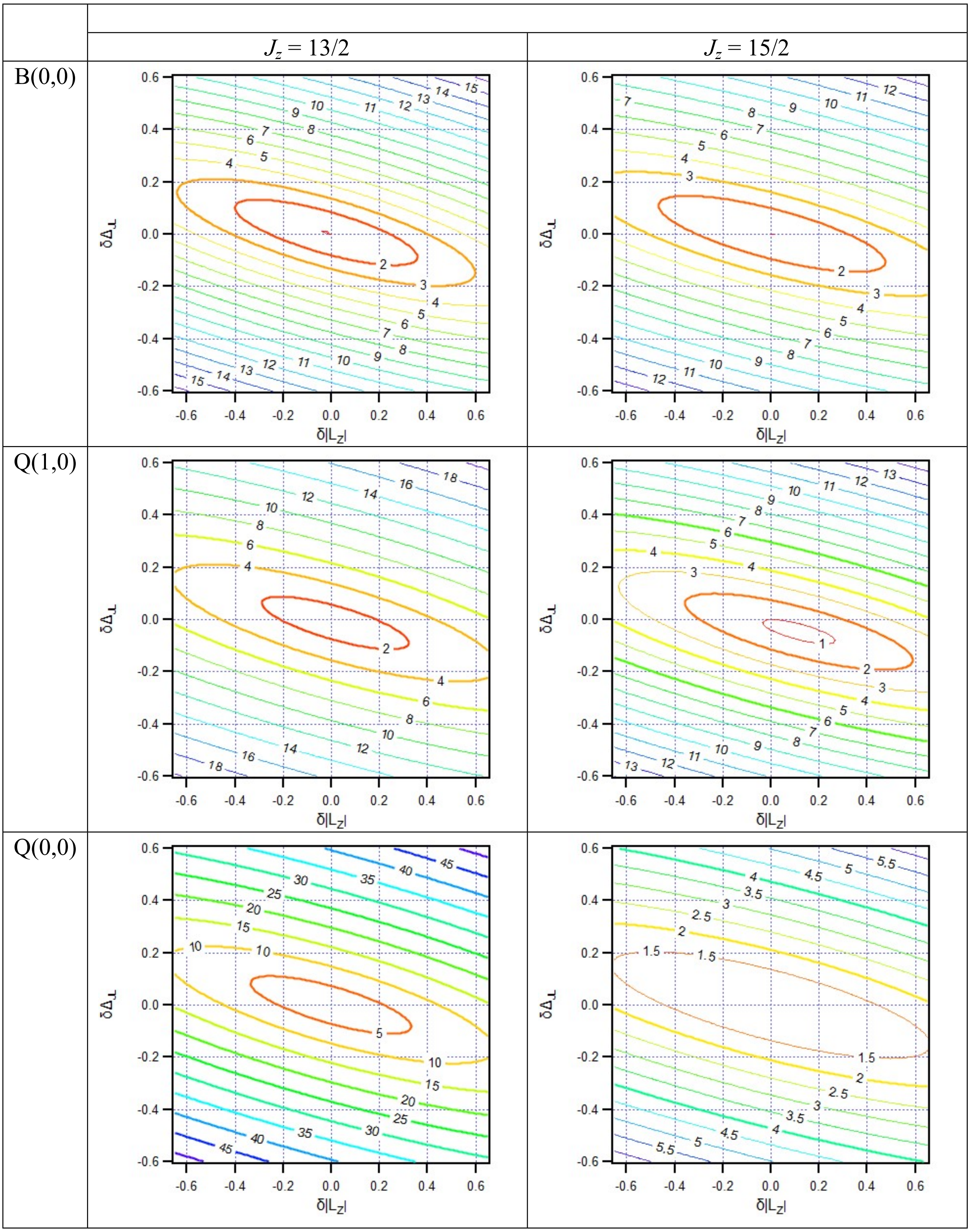


Figure S15. Contour maps of the ratio RMS1/RMS0 for $[Dy(TPP)(aza12C4)]^+$, where RMS0 is the minimum RMS error obtained with the two parameters ($|L_z|$ and Δ_{JL}) determined by means of least-square procedure, and RMS1 is the RMS error obtained varying two parameters of the two by the values indicated in the vertical and horizontal axes.

Table S1. Parameters of B and Q bands determined by the band deconvolution of absorption and MCD spectra of [Dy(TPP)(12C4)]Cl incorporated into PMMA.

		Q band					**B band**			
		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
E_0 (cm^{-1})$^{\xi}$		16940	17820	18075	18380	19520	23522	23905	24200	24700
Γ (cm^{-1})$^{\xi}$		492	420	393	555	670	431	313	500	960
η^{ξ}		0.622	0.76	0.22	0.86	0.67	0.08	0.00	0.00	0.30
D_0		0.45	0.33	0.69	1.07	0.16	22.51	2.52	0.26	3.19
Values obtained under 1 T										
T (K)		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
100	A_1/D_0	3.48136	2.65953	2.23240	0.10506	0.00000	0.29685	0.13878	0.78125	0.31369
	B_0/D_0	0.00078	0.01335	-0.00464	-0.00162	0.00000	-0.00008	0.00000	0.00000	-0.00314
1.5	A_1/D_0	2.33216	1.99032	1.47701	-0.40669	0.00000	-8.88516	-1.76705	38.28125	1.50575
	B_0/D_0	0.00894	0.01489	-0.00127	-0.00316	0.00000	-0.00027	0.00564	-0.19375	-0.00627
Values obtained at 1.5 K										
B (T)		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
1	A_1/D_0	2.33216	1.99031	1.47701	-0.40669	0.00000	-8.88516	-1.76705	38.28125	1.50575
	B_0/D_0	0.00894	0.01183	-0.00117	-0.00316	0.00000	-0.00027	0.00564	-0.19375	-0.00627
2	A_1/D_0	2.91004	2.32836	1.84483	0.29289	0.00000	-4.23276	-0.97145	31.25000	1.50575
	B_0/D_0	0.00551	0.01335	-0.00222	-0.00111	0.00000	0.00022	-0.00075	-0.10156	-0.00627
3	A_1/D_0	3.13301	2.17965	1.98731	0.29289	0.00000	-2.58865	-0.49064	19.53125	1.50575
	B_0/D_0	0.00372	0.01335	-0.00265	-0.00112	0.00000	-0.00008	-0.00075	-0.06250	-0.00627
4	A_1/D_0	3.236581	2.63255	2.06046	0.29289	0.00000	-1.81296	-0.57493	16.40625	1.50575
	B_0/D_0	0.003728	0.01395	-0.00391	-0.00111	0.00000	-0.00008	-0.00075	-0.01953	-0.00627
5	A_1/D_0	3.27301	2.48385	2.08872	0.29289	0.00000	-1.30729	-0.33703	15.625	1.50575
	B_0/D_0	0.00275	0.01335	-0.00392	-0.00111	0.00000	-0.000003	-0.00075	-0.015625	-0.00627
6	A_1/D_0	3.33468	2.48385	2.11017	0.29289	0.00000	-0.99065	-0.13877	11.71875	1.56848
	B_0/D_0	0.00227	0.01228	-0.00392	-0.00111	0.00000	-0.00003	-0.00075	-0.01172	-0.00627

Table S2. Parameters of B and Q bands determined by the band deconvolution of absorption and MCD spectra of [Dy(TPP)(aza12C4)]Cl incorporated into PMMA.

		Q band						**B band**			
		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9	Band 10
E_0 (cm^{-1})$^{\xi}$		16820	17135	18035	18275	18510	19650	23580	23902	24400	24900
Γ(cm^{-1})$^{\xi}$		280	400	485	320	460	780	613	431	400	1000
η^{ξ}		0.10	0.19	0.69	0.52	0.85	0.68	0.00	0.08	0.00	0.30
D_0		0.08	0.29	0.87	0.49	0.80	0.19	11.52	23.20	2.55	4.98
Values obtained under 1 T											
T (K)		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9	Band 10
100	A_1/D_0	3.00521	2.95580	1.47102	0.83642	-0.24924	0.00000	0.21320	0.03500	0.01262	-0.20089
	B_0/D_0	0.00128	0.00339	-0.00059	0.00366	-0.00036	0.00000	-0.00038	0.00028	-0.00038	0.00000
1.5	A_1/D_0	1.31009	-6.51392	-0.28604	-4.33780	-0.30353	0.00000	-1.77543	-12.68273	-3.53496	0.96428
	B_0/D_0	-0.02752	0.01379	-0.00265	0.00152	0.00791	0.00000	0.02592	-0.00940	-0.02570	-0.00402
Values obtained at 1.5 K											
B (T)		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9	Band 10
1	A_1/D_0	1.31009	-6.51392	-0.28604	-4.33780	-0.30353	0.00000	-1.77543	-12.68273	-3.53496	0.96428
	B_0/D_0	-0.02752	0.01379	-0.00265	0.00152	0.00791	0.00000	0.02592	-0.00940	-0.02570	-0.00402
2	A_1/D_0	0.00000	-1.69781	0.45767	-1.70857	-0.52911	0.00000	-1.32789	-6.44670	-0.86410	0.96428
	B_0/D_0	-0.02402	0.01312	-0.00250	-0.00056	0.00572	0.00000	0.01003	-0.00300	-0.01283	-0.00402
3	A_1/D_0	1.44938	0.00359	0.68650	-0.81554	0.01816	0.00000	-0.59414	-4.21795	-0.47133	0.96428
	B_0/D_0	-0.01061	0.00874	-0.00300	0.00138	0.00479	0.00000	0.00712	-0.00246	-0.00851	-0.00402
4	A_1/D_0	2.73907	0.84170	0.86957	-0.35467	0.01816	0.00000	-0.21320	-3.10455	-0.39277	0.96428
	B_0/D_0	-0.00141	0.00554	-0.00253	0.00025	0.00574	0.00000	0.00314	-0.00128	-0.00715	-0.00402
5	A_1/D_0	2.95470	1.35757	1.16430	-0.07646	-0.18165	0.00000	-0.36747	-2.43808	-0.39277	0.96428
	B_0/D_0	-0.00183	0.00527	-0.00238	-0.00049	0.00561	0.00000	0.00122	-0.00055	-0.00715	-0.00402
6	A_1/D_0	2.95470	1.68305	1.37300	0.12663	-0.26741	0.00000	-0.43531	-1.95197	0.39277	0.96428
	B_0/D_0	-0.00156	0.00544	-0.00127	-0.00193	0.00564	0.00000	-0.00132	0.00054	-0.00543	-0.00402

Table S3. L_z and Δ_{JL} values of [Dy(TPP)12C4]Cl and [Dy(TPP)aza12C4]Cl with J_z = 11/2, 13/2, and 15/2.

[Dy(TPP)(12C4)]Cl									
J_z	B(0,0)			Q(0,0)			Q(1,0)		
	L_z (ħ)	Δ_{JL} (cm^{-1})	$\Sigma Error^2$	L_z (ħ)	Δ_{JL} (cm^{-1})	$\Sigma Error^2$	L_z (ħ)	Δ_{JL} (cm^{-1})	$\Sigma Error^2$
$^{11}/_{2}$	1.18	-3.60	11.35	3.58	-0.45	0.10	2.30	-0.29	0.16
$^{13}/_{2}$	0.84	-3.19	1.1	3.53	-0.39	0.01	2.26	-0.26	0.13
[Dy(TPP)(aza12C4)]Cl									
J_z	B(0,0)			Q(0,0)			Q(1,0)		
	L_z (ħ)	Δ_{JL} (cm^{-1})	$\Sigma Error^2$	L_z (ħ)	Δ_{JL} (cm^{-1})	$\Sigma Error^2$	L_z (ħ)	Δ_{JL} (cm^{-1})	$\Sigma Error^2$
$^{11}/_{2}$	1.28	-5.25	16.72	4.23	-4.04	7.57	1.54	-2.21	3.18
$^{13}/_{2}$	0.76	-4.66	0.51	3.82	-3.58	0.04	1.32	-1.96	0.26
$^{15}/_{2}$	0.28	-4.20	0.61	3.42	-3.23	5.89	1.10	-1.76	1.47

Computational Chemistry Calculation

Table S4. Details of *ab initio* calculations

Basis Set 1	**Basis Set 2**
Dy = ANO-RCC…9s8p6d4f3g2h	Dy = ANO-RCC…8s7p5d3f2g1h
O = ANO-RCC...3s2p1d	O = ANO-RCC...3s2p1d
N = ANO-RCC...3s2p1d	N = ANO-RCC...3s2p1d
C = ANO-RCC…2s1p	C = ANO-RCC…2s1p
H = ANO-RCC…1s	H = ANO-RCC…1s

Table S5. Dipole transition strengths for [Dy(TPP)(12C4)]$^+$ obtained from CASSCF/RASSI/single_aniso calculations using Basis Set 1.

From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	282	1.41×10^{-2}	4.76×10^{6}	4.76×10^{6}	0.00	9.52×10^{6}
2	281	1.41×10^{-2}	4.76×10^{6}	4.76×10^{6}	0.00	9.52×10^{6}
1	284	1.40×10^{-2}	4.72×10^{6}	4.72×10^{6}	0.00	9.45×10^{6}
2	283	1.40×10^{-2}	4.72×10^{6}	4.72×10^{6}	0.00	9.45×10^{6}
1	813	2.84	2.20×10^{9}	2.03×10^{9}	0.00	4.24×10^{9}
2	814	2.84	2.20×10^{9}	2.03×10^{9}	0.00	4.24×10^{9}
1	817	2.44	1.76×10^{9}	1.88×10^{9}	0.00	3.64×10^{9}
2	818	2.44	1.76×10^{9}	1.88×10^{9}	0.00	3.64×10^{9}
3	285	1.41×10^{-2}	4.75×10^{6}	4.75×10^{6}	0.00	9.51×10^{6}
4	286	1.41×10^{-2}	4.75×10^{6}	4.75×10^{6}	0.00	9.51×10^{6}
3	287	1.42×10^{-2}	4.78×10^{6}	4.78×10^{6}	0.00	9.56×10^{6}
4	288	1.42×10^{-2}	4.78×10^{6}	4.78×10^{6}	0.00	9.56×10^{6}
3	824	1.94	1.53×10^{9}	1.36×10^{9}	0.00	2.90×10^{9}
4	823	1.94	1.53×10^{9}	1.36×10^{9}	0.00	2.90×10^{9}
3	826	2.98	2.11×10^{9}	2.33×10^{9}	0.00	4.44×10^{9}
4	825	2.98	2.11×10^{9}	2.33×10^{9}	0.00	4.44×10^{9}
5	277	7.95×10^{-3}	2.66×10^{6}	2.66×10^{6}	0.00	5.32×10^{6}
6	278	7.95×10^{-3}	2.66×10^{6}	2.66×10^{6}	0.00	5.32×10^{6}
5	279	7.55×10^{-3}	2.53×10^{6}	2.53×10^{6}	0.00	5.05×10^{6}
6	280	7.55×10^{-3}	2.53×10^{6}	2.53×10^{6}	0.00	5.05×10^{6}
5	820	2.86	2.29×10^{9}	1.98×10^{9}	0.00	4.27×10^{9}
6	819	2.86	2.29×10^{9}	1.98×10^{9}	0.00	4.27×10^{9}
5	822	1.79	1.20×10^{9}	1.47×10^{9}	0.00	2.67×10^{9}
6	821	1.79	1.20×10^{9}	1.47×10^{9}	0.00	2.67×10^{9}
7	289	1.39×10^{-2}	4.71×10^{6}	4.71×10^{6}	0.00	9.42×10^{6}
8	290	1.39×10^{-2}	4.71×10^{6}	4.71×10^{6}	0.00	9.42×10^{6}
7	292	1.41×10^{-2}	4.75×10^{6}	4.75×10^{6}	0.00	9.50×10^{6}
8	291	1.41×10^{-2}	4.75×10^{6}	4.75×10^{6}	0.00	9.50×10^{6}
7	828	2.71	2.39×10^{9}	1.65×10^{9}	0.00	4.05×10^{9}
8	827	2.71	2.39×10^{9}	1.65×10^{9}	0.00	4.05×10^{9}
7	830	2.70	1.64×10^{9}	2.38×10^{9}	0.00	4.02×10^{9}
8	829	2.70	1.64×10^{9}	2.38×10^{9}	0.00	4.02×10^{9}
9	294	8.07×10^{-3}	2.73×10^{6}	2.73×10^{6}	0.00	5.45×10^{6}
10	293	8.07×10^{-3}	2.73×10^{6}	2.73×10^{6}	0.00	5.45×10^{6}
9	295	7.81×10^{-3}	2.64×10^{6}	2.64×10^{6}	0.00	5.28×10^{6}
10	296	7.81×10^{-3}	2.64×10^{6}	2.64×10^{6}	0.00	5.28×10^{6}
9	832	2.62	2.48×10^{9}	1.43×10^{9}	0.00	3.91×10^{9}
10	831	2.62	2.48×10^{9}	1.43×10^{9}	0.00	3.91×10^{9}
9	834	2.73	1.50×10^{9}	2.57×10^{9}	0.00	4.07×10^{9}
10	833	2.73	1.50×10^{9}	2.57×10^{9}	0.00	4.07×10^{9}
11	301	1.49×10^{-2}	5.08×10^{6}	5.06×10^{6}	0.00	1.01×10^{7}
12	302	1.49×10^{-2}	5.08×10^{6}	5.06×10^{6}	0.00	1.01×10^{7}
11	303	1.48×10^{-2}	5.01×10^{6}	5.03×10^{6}	0.00	1.00×10^{7}
12	304	1.48×10^{-2}	5.01×10^{6}	5.03×10^{6}	0.00	1.00×10^{7}
11	836	3.02	2.34×10^{9}	2.17×10^{9}	0.00	4.51×10^{9}
12	835	3.02	2.34×10^{9}	2.17×10^{9}	0.00	4.51×10^{9}

11	837	3.00	2.16×10^{9}	2.32×10^{9}	0.00	4.47×10^{9}
12	838	3.00	2.16×10^{9}	2.32×10^{9}	0.00	4.47×10^{9}
13	297	1.50×10^{-2}	5.05×10^{6}	5.09×10^{6}	0.00	1.01×10^{7}
14	298	1.50×10^{-2}	5.05×10^{6}	5.09×10^{6}	0.00	1.01×10^{7}
13	299	1.49×10^{-2}	5.04×10^{6}	5.00×10^{6}	0.00	1.00×10^{7}
14	300	1.49×10^{-2}	5.04×10^{6}	5.00×10^{6}	0.00	1.00×10^{7}
13	839	2.98	2.77×10^{9}	1.68×10^{9}	0.00	4.45×10^{9}
14	840	2.98	2.77×10^{9}	1.68×10^{9}	0.00	4.45×10^{9}
13	842	2.97	1.69×10^{9}	2.75×10^{9}	0.00	4.44×10^{9}
14	841	2.97	1.69×10^{9}	2.75×10^{9}	0.00	4.44×10^{9}
15	274	1.52×10^{-2}	4.97×10^{6}	4.97×10^{6}	0.00	9.95×10^{6}
16	273	1.52×10^{-2}	4.97×10^{6}	4.97×10^{6}	0.00	9.95×10^{6}
15	276	1.51×10^{-3}	4.95×10^{6}	4.95×10^{6}	0.00	9.91×10^{6}
16	275	1.51×10^{-3}	4.95×10^{6}	4.95×10^{6}	0.00	9.91×10^{6}
15	843	2.98	2.79×10^{9}	1.66×10^{9}	0.00	4.45×10^{9}
16	844	2.98	2.79×10^{9}	1.66×10^{9}	0.00	4.45×10^{9}
15	845	2.99	1.66×10^{9}	2.81×10^{9}	0.00	4.47×10^{9}
16	846	2.99	1.66×10^{9}	2.81×10^{9}	0.00	4.47×10^{9}

Table S6. Dipole transition strengths for $[Dy(TPP)(aza12C4)]^{+}$ obtained from CASSCF/RASSI/single_aniso calculations using Basis Set 1.

From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	265	2.95×10^{-3}	1.78×10^{6}	1.79×10^{5}	2.17×10^{1}	1.96×10^{6}
2	266	2.95×10^{-3}	1.78×10^{6}	1.79×10^{5}	2.17×10^{1}	1.96×10^{6}
1	283	5.35×10^{-3}	1.08×10^{6}	2.51×10^{6}	4.33×10^{1}	3.59×10^{6}
2	284	5.35×10^{-3}	1.08×10^{6}	2.51×10^{6}	4.33×10^{1}	3.59×10^{6}
1	805	2.11	1.60×10^{9}	1.49×10^{9}	8.97×10^{3}	3.09×10^{9}
2	806	2.11	1.60×10^{9}	1.49×10^{9}	8.97×10^{3}	3.09×10^{9}
1	819	1.90	1.35×10^{9}	1.46×10^{9}	1.42×10^{4}	2.81×10^{9}
2	820	1.90	1.35×10^{9}	1.46×10^{9}	1.42×10^{4}	2.81×10^{9}
3	271	2.30×10^{-3}	1.35×10^{6}	1.80×10^{5}	1.52×10^{1}	1.53×10^{6}
4	272	2.30×10^{-3}	1.35×10^{6}	1.80×10^{5}	1.52×10^{1}	1.53×10^{6}
3	285	6.70×10^{-3}	1.28×10^{6}	3.22×10^{6}	3.66×10^{1}	4.49×10^{6}
4	286	6.70×10^{-3}	1.28×10^{6}	3.22×10^{6}	3.66×10^{1}	4.49×10^{6}
3	807	2.90	2.24×10^{9}	2.00×10^{9}	1.24×10^{4}	4.23×10^{9}
4	808	2.90	2.24×10^{9}	2.00×10^{9}	1.24×10^{4}	4.23×10^{9}
3	821	1.42	9.86×10^{8}	1.12×10^{9}	1.07×10^{1}	2.11×10^{9}
4	822	1.42	9.86×10^{8}	1.12×10^{9}	1.07×10^{1}	2.11×10^{9}
5	276	3.26×10^{-3}	1.92×10^{6}	2.50×10^{5}	1.62×10^{1}	2.17×10^{6}
6	275	3.26×10^{-3}	1.92×10^{6}	2.50×10^{5}	1.62×10^{1}	2.17×10^{6}
5	288	4.07×10^{-3}	7.87×10^{5}	1.95×10^{6}	2.29×10^{1}	2.73×10^{6}
6	287	4.07×10^{-3}	7.87×10^{5}	1.95×10^{6}	2.29×10^{1}	2.73×10^{6}
5	810	2.33	1.80×10^{9}	1.60×10^{9}	9.85×10^{3}	3.40×10^{9}
6	809	2.33	1.80×10^{9}	1.60×10^{9}	9.85×10^{3}	3.40×10^{9}
5	826	2.34	1.65×10^{9}	1.81×10^{9}	1.74×10^{4}	3.47×10^{9}
6	825	2.34	1.65×10^{9}	1.81×10^{9}	1.74×10^{4}	3.47×10^{9}

7	280	2.65×10^{-3}	1.56×10^{6}	2.07×10^{5}	1.13×10^{1}	1.76×10^{6}
8	279	2.65×10^{-3}	1.56×10^{6}	2.07×10^{5}	1.13×10^{1}	1.76×10^{6}
7	292	2.30×10^{-3}	4.22×10^{5}	1.12×10^{6}	1.23×10^{1}	1.54×10^{6}
8	291	2.30×10^{-3}	4.22×10^{5}	1.12×10^{6}	1.23×10^{1}	1.54×10^{6}
7	812	2.19	1.68×10^{9}	1.52×10^{9}	9.04×10^{3}	3.20×10^{9}
8	811	2.19	1.68×10^{9}	1.52×10^{9}	9.04×10^{3}	3.20×10^{9}
7	828	2.01	1.41×10^{9}	1.56×10^{9}	1.53×10^{4}	2.98×10^{9}
8	827	2.01	1.41×10^{9}	1.56×10^{9}	1.53×10^{4}	2.98×10^{9}
9	281	3.42×10^{-3}	2.02×10^{6}	2.50×10^{5}	8.16×10^{0}	2.27×10^{6}
10	282	3.42×10^{-3}	2.02×10^{6}	2.50×10^{5}	8.16×10^{0}	2.27×10^{6}
9	295	6.00×10^{-3}	1.16×10^{6}	2.86×10^{6}	2.81×10^{1}	4.03×10^{6}
10	296	6.00×10^{-3}	1.16×10^{6}	2.86×10^{6}	2.81×10^{1}	4.03×10^{6}
9	813	2.83	2.17×10^{9}	1.96×10^{9}	1.15×10^{4}	4.13×10^{9}
10	814	2.83	2.17×10^{9}	1.96×10^{9}	1.15×10^{4}	4.13×10^{9}
9	831	2.90	2.04×10^{9}	2.25×10^{9}	2.19×10^{4}	4.29×10^{9}
10	832	2.90	2.04×10^{9}	2.25×10^{9}	2.19×10^{4}	4.29×10^{9}
11	289	3.22×10^{-3}	1.93×10^{6}	2.11×10^{5}	1.72×10^{1}	2.14×10^{6}
12	290	3.22×10^{-3}	1.93×10^{6}	2.11×10^{5}	1.72×10^{1}	2.14×10^{6}
11	300	7.20×10^{-3}	1.41×10^{6}	3.42×10^{6}	3.96×10^{1}	4.83×10^{6}
12	299	7.20×10^{-3}	1.41×10^{6}	3.42×10^{6}	3.96×10^{1}	4.83×10^{6}
11	815	2.99	2.31×10^{9}	2.07×10^{9}	1.26×10^{4}	4.38×10^{9}
12	816	2.99	2.31×10^{9}	2.07×10^{9}	1.26×10^{4}	4.38×10^{9}
11	840	3.04	2.14×10^{9}	2.36×10^{9}	2.30×10^{4}	4.50×10^{9}
12	839	3.04	2.14×10^{9}	2.36×10^{9}	2.30×10^{4}	4.50×10^{9}
13	291	2.06×10^{-3}	1.22×10^{6}	1.46×10^{5}	1.03×10^{1}	1.37×10^{6}
14	292	2.06×10^{-3}	1.22×10^{6}	1.46×10^{5}	1.03×10^{1}	1.37×10^{6}
13	294	1.32×10^{-3}	7.64×10^{5}	1.17×10^{5}	7.45×10^{0}	8.80×10^{5}
14	293	1.32×10^{-3}	7.64×10^{5}	1.17×10^{5}	7.45×10^{0}	8.80×10^{5}
13	817	2.80	2.14×10^{9}	1.95×10^{9}	1.15×10^{4}	4.09×10^{9}
14	818	2.80	2.14×10^{9}	1.95×10^{9}	1.15×10^{4}	4.09×10^{9}
13	843	3.07	2.17×10^{9}	2.37×10^{9}	2.31×10^{4}	4.54×10^{9}
14	844	3.07	2.17×10^{9}	2.37×10^{9}	2.31×10^{4}	4.54×10^{9}
15	297	3.21×10^{-3}	1.90×10^{6}	2.33×10^{5}	1.20×10^{1}	2.13×10^{6}
16	298	3.21×10^{-3}	1.90×10^{6}	2.33×10^{5}	1.20×10^{1}	2.13×10^{6}
15	303	7.31×10^{-3}	1.42×10^{6}	3.49×10^{6}	3.98×10^{1}	4.91×10^{6}
16	304	7.31×10^{-3}	1.42×10^{6}	3.49×10^{6}	3.98×10^{1}	4.91×10^{6}
15	821	1.53	1.18×10^{9}	1.06×10^{9}	6.39×10^{3}	2.24×10^{9}
16	822	1.53	1.18×10^{9}	1.06×10^{9}	6.39×10^{3}	2.24×10^{9}
15	846	3.08	2.17×10^{9}	2.39×10^{9}	2.32×10^{4}	4.56×10^{9}
16	845	3.08	2.17×10^{9}	2.39×10^{9}	2.32×10^{4}	4.56×10^{9}

Table S7. The calculated transition energy, orbital and spin angular momenta of the ground doublet and the excited doublet SO states for $[Dy(TPP)(12C4)]^+$, generated from CAS(11,13) calculation with basis set 1.

Doublet	Spin-orbit State	Energy (cm^{-1})	initial doublet → final doublet	$\|L_z\|$	$\|S_z\|$	$\|J_z\|$ = $\|L_z+S_z\|$	Change in $\|J_z\|$ from the initial doublet	Primal $\|J_z\rangle$	Δ_{JL}
1	1, 2	0.000		2.91	1.48	4.39		0.80 $\|\pm 11/2\rangle$, 0.13 $\|\pm 3/2\rangle$	
2	3, 4	17.387		1.27	0.62	1.89		0.57 $\|\pm 9/2\rangle$, 0.22 $\|\pm 11/2\rangle$, 0.21 $\|\pm 1/2\rangle$	
3	5, 6	47.144		1.83	0.96	2.79		0.42 $\|\pm 13/2\rangle$, 0.35 $\|\pm 5/2\rangle$, 0.12 $\|\pm 11/2\rangle$ 0.10 $\|\pm 3/2\rangle$	
4	7, 8	65.885		0.32	0.17	0.49		0.60 $\|\pm 7/2\rangle$, 0.35 $\|\pm 9/2\rangle$	
5	9,10	78.945		2.41	1.25	3.66		0.56 $\|\pm 13/2\rangle$, 0.22 $\|\pm 5/2\rangle$, 0.17 $\|\pm 3/2\rangle$	
6	11,12	203.961		0.06	0.01	0.07		0.60 $\|\pm 3/2\rangle$, 0.36 $\|\pm 5/2\rangle$	
7	13,14	217.607		0.07	0.02	0.09		0.75 $\|\pm 1/2\rangle$, 0.17 $\|\pm 7/2\rangle$	
8	15, 16	340.158		4.98	2.50	7.48		1.00 $\|\pm 15/2\rangle$	
137	273, 274	31696.829	8→137	9.53	2.50	12.03	+4.55		5.83
138	275, 276	31708.494	8→138	0.41	2.49	2.90	−4.58		
139	277, 278	31724.052	3→139	0.29	2.14	1.85	−0.94		−4.60
140	279, 280	31733.254	3→140	8.84	2.14	10.98	+8.19		
141	281, 282	31769.706	1→141	1.06	1.72	0.66	−3.73		−5.55
142	283, 284	31780.817	1→142	8.07	1.74	9.81	+5.42		
143	285, 286	31811.562	2→143	2.29	1.10	1.20	−0.69		−2.85
144	287, 288	31817.267	2→144	6.76	1.09	7.85	+5.96		
145	289, 290	31882.624	4→145	3.39	0.51	2.88	2.39		0.75
146	291, 292	31884.116	4→146	5.86	0.62	6.48	5.99		
147	293, 294	31911.725	5→147	4.07	0.18	3.89	0.23		0.12
148	295, 296	31911.958	5→148	5.14	0.27	5.41	1.75		

149	297, 298	32037.810	7→149	4.47	0.04	4.43	4.34		0.09
150	299, 300	32037.984	7→150	4.32	0.05	4.27	4.18		
151	301, 302	32057.291	6→151	4.46	0.04	4.42	4.35		0.19
152	303, 304	32057.667	6→152	4.29	0.07	4.22	4.15		
407	813, 814	47287.937	1→ 407	2.64	1.40	4.04	−0.35		
409	817, 818	47298.759	1→ 409	1.20	0.61	1.81	−2.58		
412	823, 824	47314.291	2→ 412	2.13	1.12	3.25	1.36		
413	825, 826	47322.772	2→ 413	3.88	1.92	5.80	3.91		
410	819, 820	47305.244	3→ 410	0.04	0.02	0.06	−2.73		
411	821,822	47309.567	3→ 411	1.89	0.97	2.86	0.07		
414	827, 828	47361.818	4→ 414	2.25	1.16	3.41	2.92		
415	829, 830	47364.496	4→ 415	2.05	1.05	3.10	2.61		
416	831, 832	47371.187	5→ 416	2.49	1.27	3.76	0.10		
417	833, 834	47373.110	5→ 417	2.76	1.41	4.17	0.51		
418	835, 836	47451.018	6→ 418	5.08	2.48	7.56	7.49		
419	837, 838	47465.220	6→ 419	4.67	2.41	7.08	7.01		
420	839, 840	47506.595	7→ 420	0.09	0.02	0.11	0.02		
421	841, 842	47508.637	7→ 421	0.11	0.07	0.18	0.09		
422	843, 844	47510.110	8→ 422	0.04	0.02	0.06	−7.42		
423	845, 846	47512.071	8→ 423	0.04	0.02	0.06	−7.42		

Table S8. The calculated transition energy, orbital and spin angular momenta of the ground doublet and the excited doublet SO states for [Dy(TPP)(aza12C4)]$^+$, generated from CAS(11,13) calculation with basis set 1.

Doublet	Spin-orbit State	Energy (cm^{-1})	Transition (initial doublet → final doublet)	$\vert L_z\vert$	$\vert S_z\vert$	$\vert J_z\vert = \vert L_z+S_z\vert$	Change in $\vert J_z\vert$ from the initial doublet	Primal $\vert J_z\rangle$	Δ_{JL}
1	1, 2	0.000		4.52	2.28	6.80		0.73 $\vert \pm 15/2\rangle$ 0.11 $\vert \pm 11/2\rangle$	
2	3, 4	34.333		3.59	1.80	5.39		0.47 $\vert \pm 13/2\rangle$ 0.16 $\vert \pm 9/2\rangle$	
3	5, 6	77.979		2.93	1.46	4.39		0.26 $\vert \pm 5/2\rangle$ 0.21 $\vert \pm 13/2\rangle$	
4	7, 8	118.022		0.60	0.30	0.90		0.30 $\vert \pm 11/2\rangle$ 0.29 $\vert \pm 3/2\rangle$	

5	9, 10	136.728		3.34	1.70	5.04		0.48 $\vert\pm 1/2\rangle$ 0.18 $\vert\pm 3/2\rangle$
6	11, 12	250.440		4.66	2.34	7.00		0.25 $\vert\pm 9/2\rangle$ 0.21 $\vert\pm 11/2\rangle$
7	13, 14	271.626		4.61	2.31	6.92		0.27 $\vert\pm 5/2\rangle$ 0.20 $\vert\pm 3/2\rangle$
8	15, 16	295.791		4.81	2.41	7.22		0.31 $\vert\pm 7/2\rangle$ 0.24 $\vert\pm 9/2\rangle$
133	265, 266	31568.164	1→133	4.33	2.22	6.55	−0.25	
142	283, 284	31723.432	1→142	4.57	2.24	6.81	+0.01	
136	271, 272	31600.921	2→136	3.23	1.44	4.67	−0.72	
143	285, 286	31753.950	2→143	3.67	1.83	5.50	+0.11	
138	275, 276	31647.656	3→138	3.00	1.47	4.47	+0.08	
144	287, 288	31800.946	3→144	2.96	1.49	4.45	+0.06	
140	279, 280	31687.834	4→140	0.87	0.44	1.31	+0.41	
147	293, 294	31844.224	4→147	2.70	1.37	4.07	+3.17	
141	281, 282	31711.602	5→141	3.34	1.81	5.15	+0.11	
148	295, 296	31865.315	5→148	3.77	1.82	5.59	+0.55	
145	289, 290	31821.021	6→145	4.64	2.30	6.94	−0.06	
150	299, 300	31972.750	6→150	4.74	2.40	7.14	+0.14	
146	291, 292	31838.455	7→146	3.31	1.67	4.98	−1.94	
151	301, 302	31996.565	7→151	4.69	2.35	7.04	+0.12	
149	297, 298	31872.145	8→149	4.99	2.34	7.33	+0.11	
152	303, 304	32025.218	8→152	4.51	2.42	6.93	−0.29	
403	805, 806	46814.924	1→ 403	4.48	2.26	6.74	−0.06	
410	819, 820	47091.223	1→ 410	4.30	2.17	6.47	−0.33	
404	807, 808	46846.210	2→ 404	3.70	1.86	5.56	+0.17	
411	821, 822	47119.802	2→ 411	3.45	1.73	5.18	−0.12	
405	809, 810	46894.888	3→ 405	3.01	1.49	4.50	+0.11	
413	825, 826	47168.618	3→ 413	2.96	1.47	4.43	+0.04	
406	811, 812	46935.309	4→ 406	2.22	1.10	3.32	+2.42	
414	827, 828	47207.877	4→ 414	0.94	0.47	1.41	+0.51	
407	813, 814	46960.985	5→ 407	3.50	1.79	5.29	+0.25	
416	831, 832	47234.112	5→ 416	3.63	1.86	5.49	+0.45	
408	815, 816	47067.566	6→ 408	4.74	2.38	7.12	+0.12	
420	839, 840	47340.180	6→ 420	4.78	2.40	7.18	+0.18	
409	817, 818	47086.990	7→ 409	4.54	2.28	6.82	−0.10	
422	843, 844	47362.923	7→ 422	4.72	2.37	7.09	+0.17	
411	821, 822	47119.802	8→ 411	3.45	1.73	5.18	−2.04	

423	845, 846	47394.809	8→ 423	4.85	2.44	7.29	+0.07

Optimized structure of $[Y(TPP)(12C4)]^+$

Y 0. 0. -0.068914911

N 1.4744075927 1.4732339496 -1.1475352824

N -1.4732339496 1.4744075927 -1.1475352824

N -1.4744075927 -1.4732339496 -1.1475352824

N 1.4732339496 -1.4744075927 -1.1475352824

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C 0.0013808993 3.4681721947 -1.3503275751

C -3.4681721947 0.0013808993 -1.3503275751

C -0.0013808993 -3.4681721947 -1.3503275751

C 2.8260482959 1.2558096718 -1.3168433127

C -1.2558096718 2.8260482959 -1.3168433127

C -2.8260482959 -1.2558096718 -1.3168433127

C 1.2558096718 -2.8260482959 -1.3168433127

C 1.2580597313 2.825047365 -1.3168433127

C -2.825047365 1.2580597313 -1.3168433127

C -1.2580597313 -2.825047365 -1.3168433127

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C 3.4897559911 2.5227405505 -1.5380279686

C 2.5255187365 3.4877459589 -1.5380279686

C 3.4877459589 -2.5255187365 -1.5380279686

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C -2.5227405505 3.4897559911 -1.5380279686

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H 4.5485048394 2.6493037787 -1.7136156416

H 2.6529250346 4.5463936859 -1.7136156416

H -2.6493037787 4.5485048394 -1.7136156416

H	-4.5463936859	2.6529250346	-1.7136156416
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H	-0.0035133931	-8.8239978814	-2.0571176352
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H	0.0035133931	8.8239978814	-2.0571176352
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C	0.0021933964	5.508784371	-2.8363536119
C	0.0019745916	4.9592493283	-1.5453312782
C	0.0023199798	5.8267025228	-0.4436701746
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C	-7.7472144176	0.0030846574	-1.9142009807
H	-8.8239978814	0.0035133931	-2.0571176352
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C	-5.8267025228	0.0023199798	-0.4436701746
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C	7.7472144176	-0.0030846574	-1.9142009807
H	8.8239978814	-0.0035133931	-2.0571176352
C	6.8928813159	-0.0027444932	-3.0190128163
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H	-2.6882311079	1.0615505239	3.2170392544
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H	-1.0615505239	-2.6882311079	3.2170392544
H	1.0594094771	-2.6890755965	3.2170392544
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H	2.6890755965	1.0594094771	3.2170392544
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H	-3.1671220938	1.524993892	1.5670564814
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H	-1.524993892	-3.1671220938	1.5670564814
H	1.5224713446	-3.168335483	1.5670564814
H	3.1671220938	-1.524993892	1.5670564814
H	3.168335483	1.5224713446	1.5670564814
H	-0.0031334228	-7.8696902758	0.2392103866
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H	-5.4146501014	0.0021559156	0.562859739
H	-7.8696902758	0.0031334228	0.2392103866
H	-7.3028781963	0.0029077389	-4.0250727128

H	-4.8457018572	0.0019293812	-3.6971827946
H	7.3028781963	-0.0029077389	-4.0250727128
H	7.8696902758	-0.0031334228	0.2392103866
H	5.4146501014	-0.0021559156	0.562859739
H	4.8457018572	-0.0019293812	-3.6971827946
H	0.0031334228	7.8696902758	0.2392103866
H	0.0021559156	5.4146501014	0.562859739
H	0.0029077389	7.3028781963	-4.0250727128
H	0.0019293812	4.8457018572	-3.6971827946

Optimized structure of $[Y(TPP)(aza12C4)]^+$

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N	-2.0751576849	-0.0308687446	-1.142781683
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C	1.1382657107	-2.8846262135	-1.322903711
C	2.9043760232	-1.0940818076	-1.2997204015
C	2.4402769106	2.4654047293	-1.2929491491
C	2.4823089691	-2.4432228933	-1.3549350215
C	-2.4279488619	-2.4895873575	-1.3058130394
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C	0.6517588079	4.2467872458	-1.5000607223
C	-0.7118125335	4.2281116288	-1.5347363593

C	-4.2550827262	0.6276803424	-1.4982421059
C	-4.2419478847	-0.736446741	-1.4873588747
C	-0.6409170591	-4.2694756217	-1.5022498109
C	0.7219746819	-4.2536383704	-1.5350494648
C	4.2692769436	-0.6498902247	-1.478647189
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H	-1.290571321	-5.1198756138	-1.6486647966
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H	5.1211396066	-1.2946099547	-1.63802311
H	1.2999317858	5.098303026	-1.6463628002
H	-1.3753328317	5.0598448843	-1.7216931434
H	-5.1061436873	1.2739224385	-1.655248537
H	-5.077948967	-1.4031112921	-1.6415452696
N	1.3066215914	-1.5613856085	1.6904065229
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C	-2.0819881513	0.9336753906	2.7205637846
C	-2.5744376187	-0.3966764234	2.174639583
C	-0.8795219608	-2.027713693	2.749271966
C	0.4079866957	-2.620835322	2.1954050931
H	2.9234827866	-1.4595097995	3.1014227052
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H	-0.6910603969	-1.4400179498	3.6581653154
H	-1.5113502876	0.7920996376	3.6484047509
H	3.2366296425	0.3473564936	1.3558695827

H	-0.2705514754	3.2337459963	1.2577807632
H	-3.1988798618	-0.2424177086	1.2929336231
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H	-0.9853919696	3.2239095575	2.886715603
H	-3.1569571645	-0.935667619	2.9309967374
H	0.8800014989	-3.2318806716	2.9796724412
H	1.9637200104	-1.9904064516	1.0366702704
H	-4.18357741	-3.3477912289	0.5821709313
C	-4.3142947466	-3.8696232187	-0.3625405127
C	-5.3015732523	-4.8487540543	-0.4855562002
H	-5.9349021541	-5.0870836663	0.3645482978
C	-5.4738319398	-5.5201742471	-1.6976250977
H	-6.2428769785	-6.2810743596	-1.7952292202
C	-4.6551225351	-5.2060194731	-2.7843665295
H	-4.7881979371	-5.7185169951	-3.7329925675
C	-3.6666892219	-4.2280911454	-2.6602645258
H	-3.0376274264	-3.9798454175	-3.5106238388
C	-3.4817664834	-3.5490528608	-1.4456285116
H	5.9484268261	5.0604788294	0.3794049173
C	5.3138503247	4.8241188259	-0.4703643874
C	4.3287165933	3.8425300005	-0.3490194625
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C	3.6759280723	4.208357038	-2.6441762594
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H	4.7921710807	5.7050439723	-3.7135580788
C	5.4821975031	5.5005930073	-1.6801296054
H	6.2492172237	6.2637432517	-1.7763462074
H	-3.3299275688	4.2646578279	0.4388525712
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C	-4.8265382109	5.3293713729	-0.6877982645
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H	-6.2539157309	6.2059084417	-2.0468566557
C	-5.1754529324	4.572187678	-2.95379614
H	-5.6843424892	4.6588444928	-3.909678933
C	-4.1984512269	3.5910745858	-2.7778862559
H	-3.9473593217	2.9212553966	-3.5956673389
C	-3.523623847	3.4651537137	-1.5532673673
H	5.1177490701	-6.0565796664	0.0266587387
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C	3.8848513263	-4.3918654211	-0.5604849398
H	3.3864604555	-4.3315158816	0.4044452911
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H	3.9181902002	-2.9081844068	-3.6170255633
C	5.1601976146	-4.5692720467	-3.0316919894
H	5.6485879548	-4.637927711	-3.9996141679
C	5.500598073	-5.4586056259	-2.0101841871
H	6.2581577078	-6.2186372875	-2.1780510726