Electronic Supplementary Information

Magnetic interaction in photoexcited terbium-porphyrin complexes with non-aromatic ligands having different symmetries

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Keywords : magnetic interaction, ferromagnetic, electronic structure and monoporphyrinato

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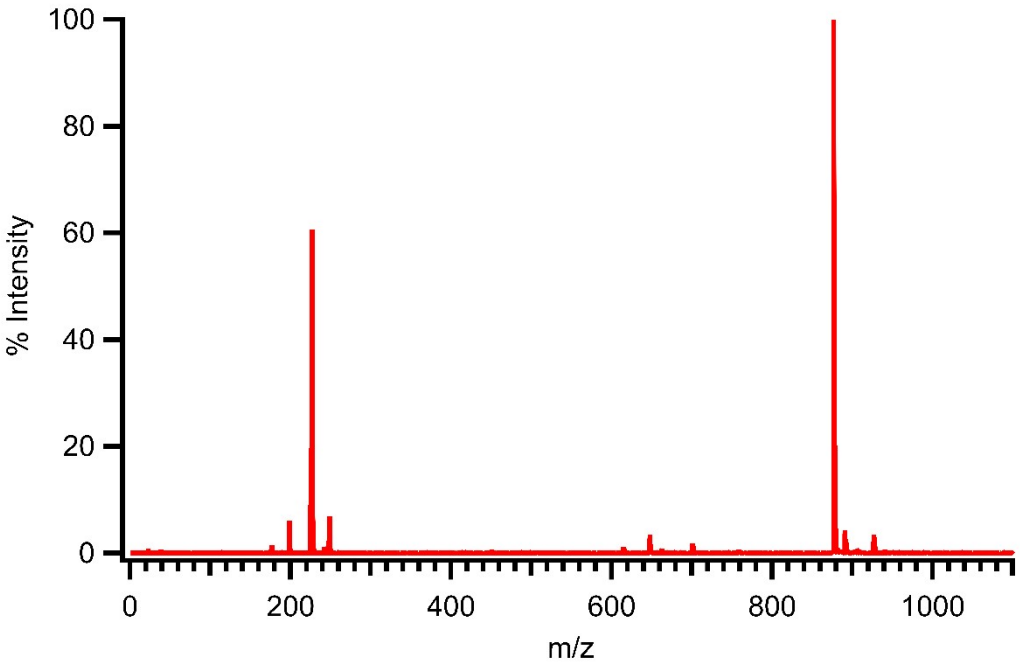

Figure S1. MALDI-TOF spectra of $[Y(TPP)(12C4)]^+$ with dithranol as matrix ($C_{14}H_{10}O_3$)at m/z equal 227.07.

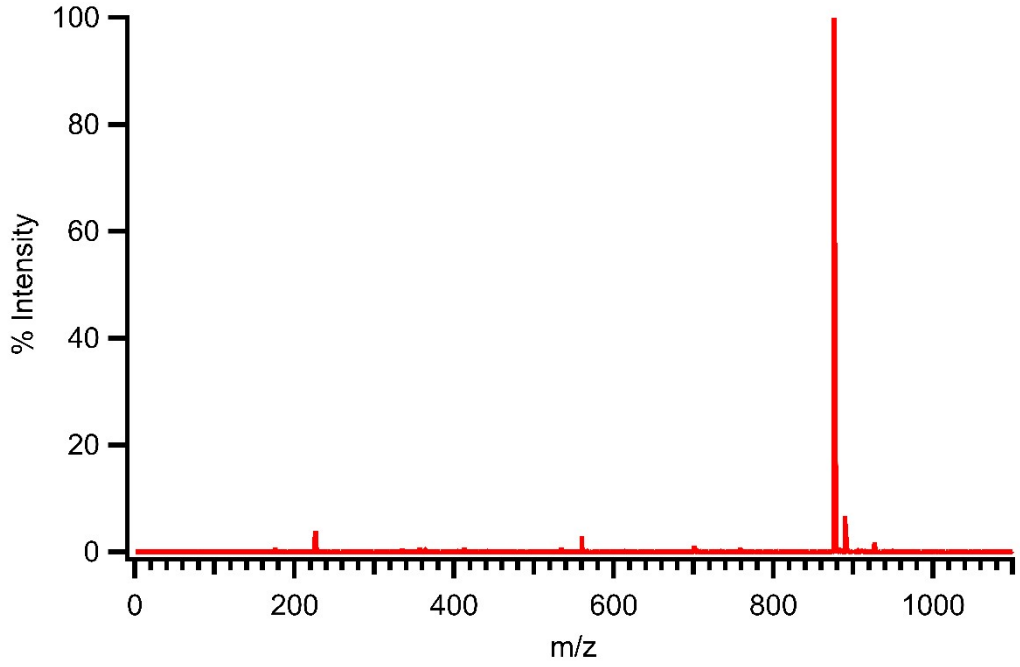

Figure S2. MALDI-TOF spectra of $[Y(TPP)(aza12C4)]^+$ with dithranol as matrix ($C_{14}H_{10}O_3$)at m/z equal 227.06.

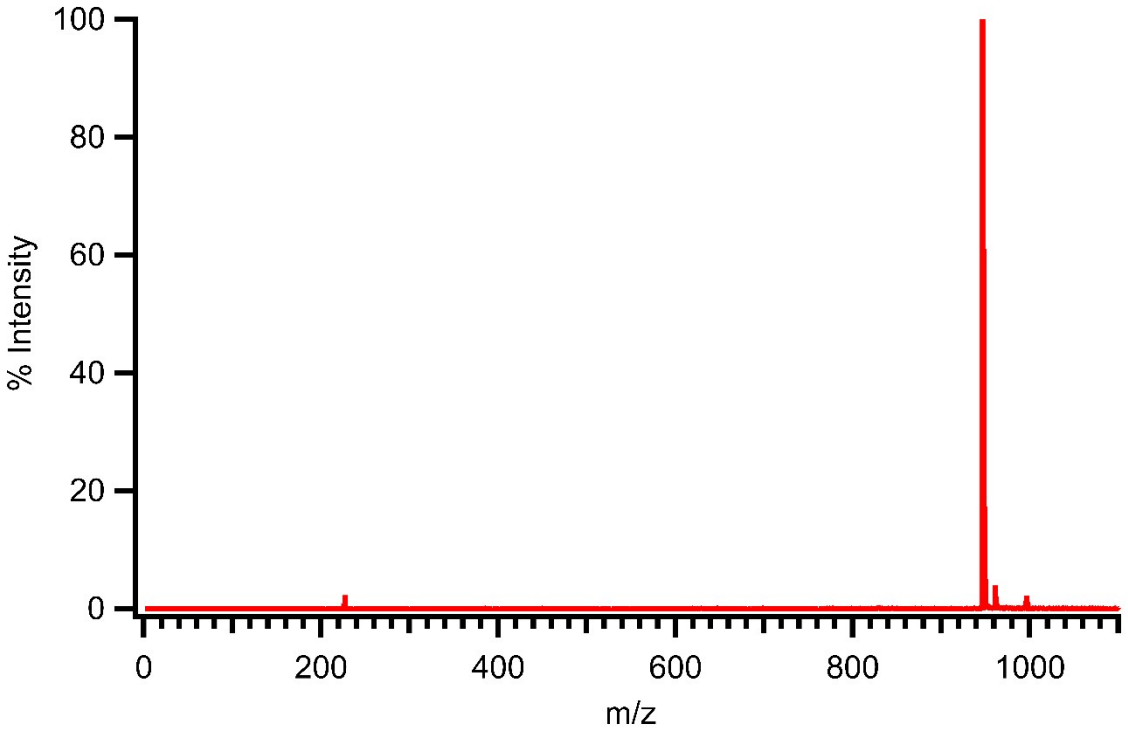

Figure S3. MALDI-TOF spectra of $[Tb(TPP)(12C4)]^+$ with dithranol as matrix ($C_{14}H_{10}O_3$) at m/z equal 227.06.

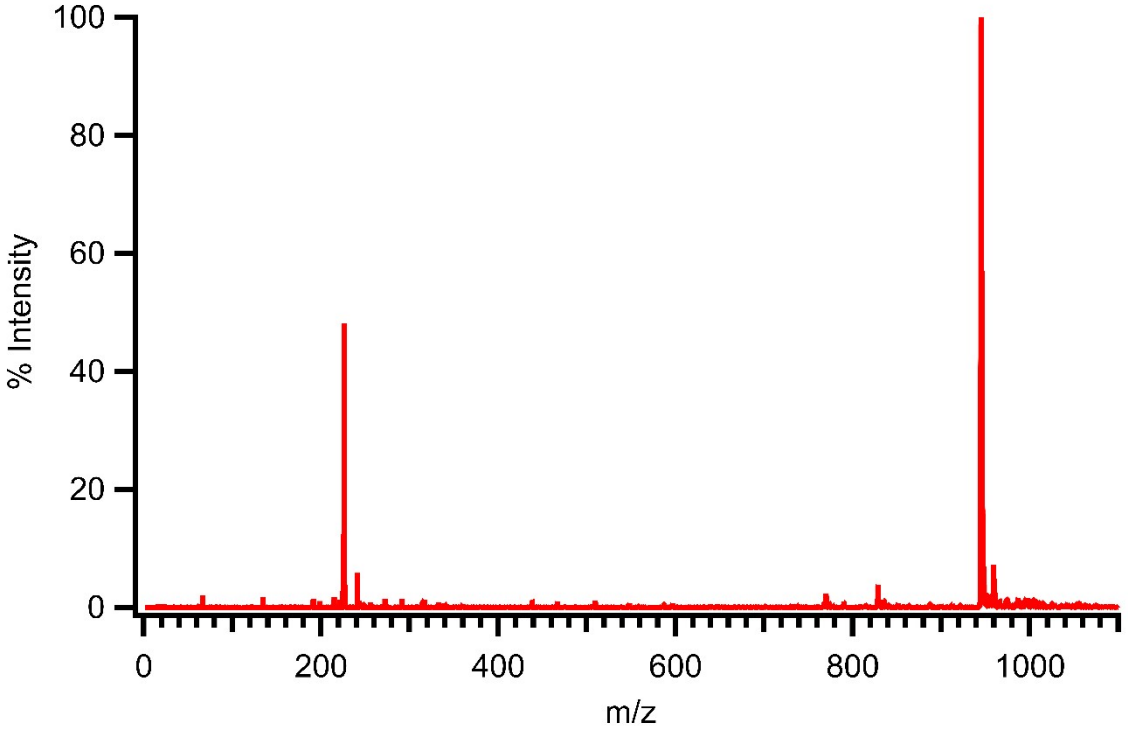

Figure S4. MALDI-TOF spectra of $[Tb(TPP)(aza12C4)]^+$ with dithranol as matrix ($C_{14}H_{10}O_3$)at m/z equal 227.06.

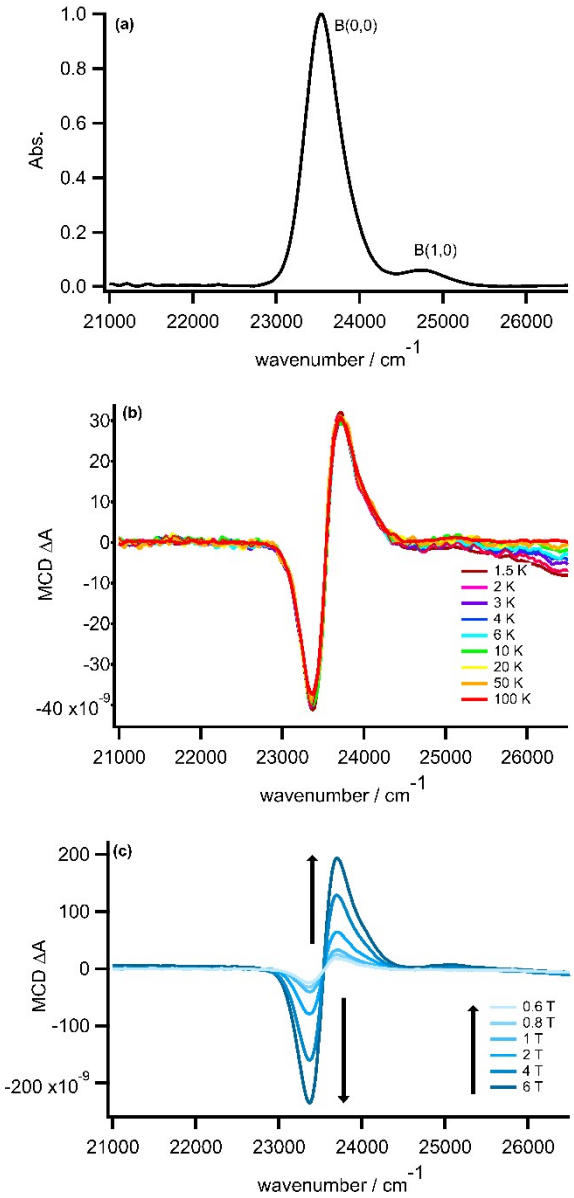

Figure S5. **(a)** Absorption, **(b)** temperature-dependent MCD spectra measured at temperatures of 1.5-100 K under a magnetic field of 1 T, and **(c)** magnetic field-dependent MCD spectra measured at temperatures of 1.5 K of B band in [Y(TPP)(12C4)]Cl in PMMA film.

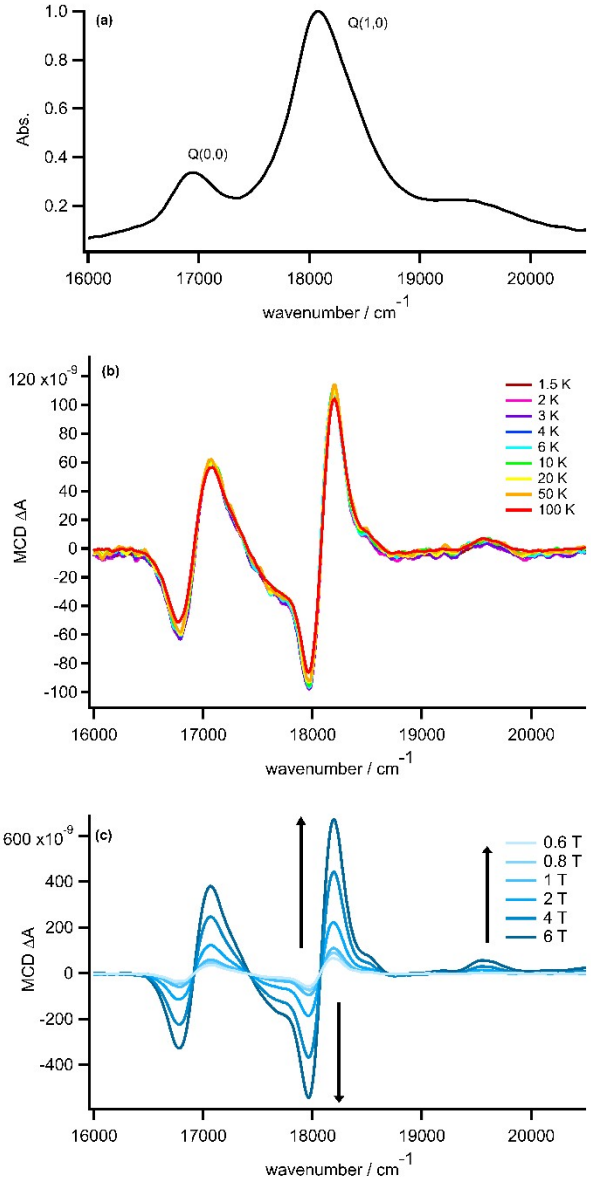

Figure S6. **(a)** Absorption, **(b)** temperature-dependent MCD spectra measured at temperatures of 1.5-100 K under a magnetic field of 1 T, and **(c)** magnetic field-dependent MCD spectra measured at temperatures of 1.5 K of Q band in [Y(TPP)(12C4)]Cl in PMMA film.

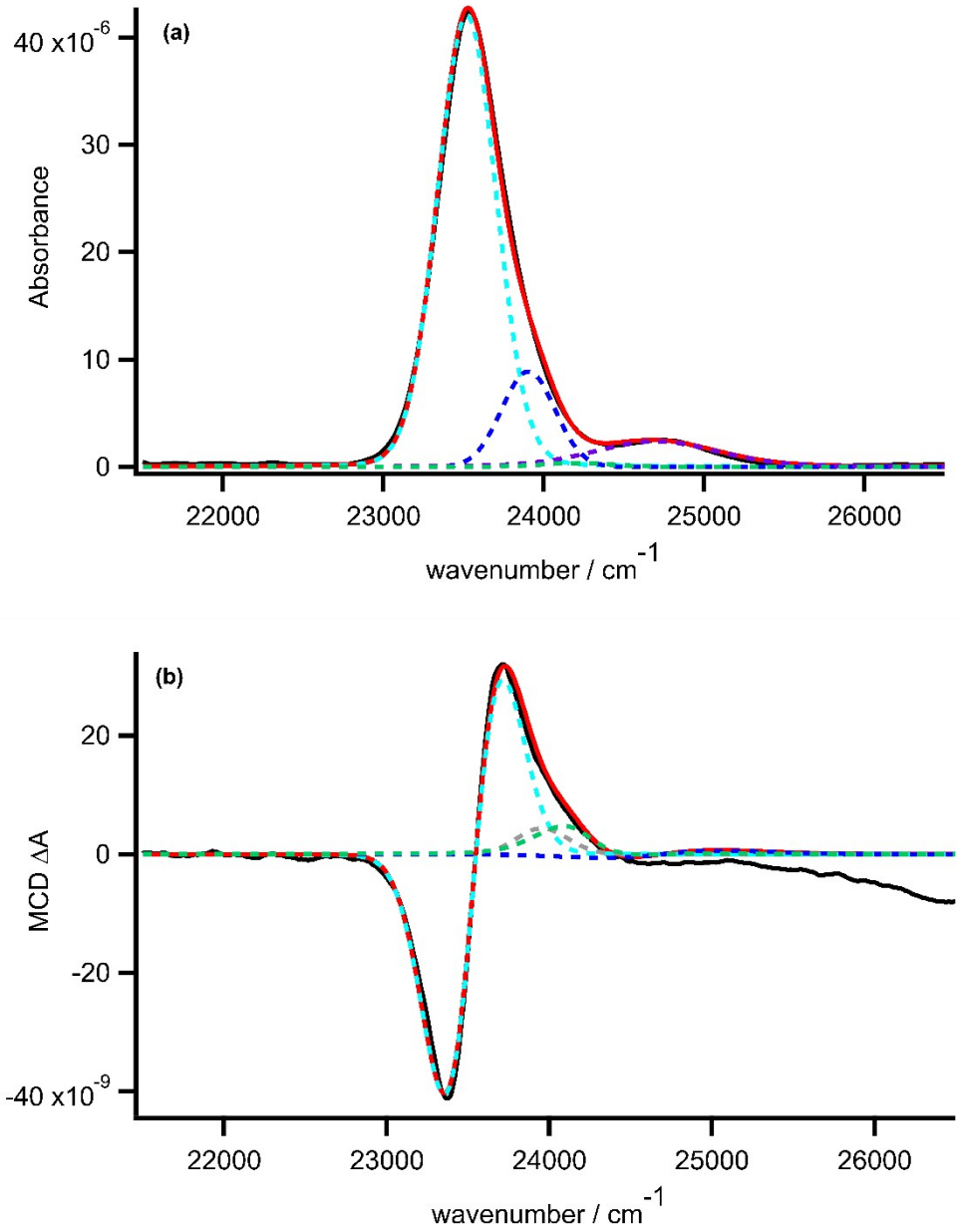

Figure S7. Band deconvolution of absorption (**a**) and MCD (**b**) of B(0,0) band spectra [Y(TPP)(12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

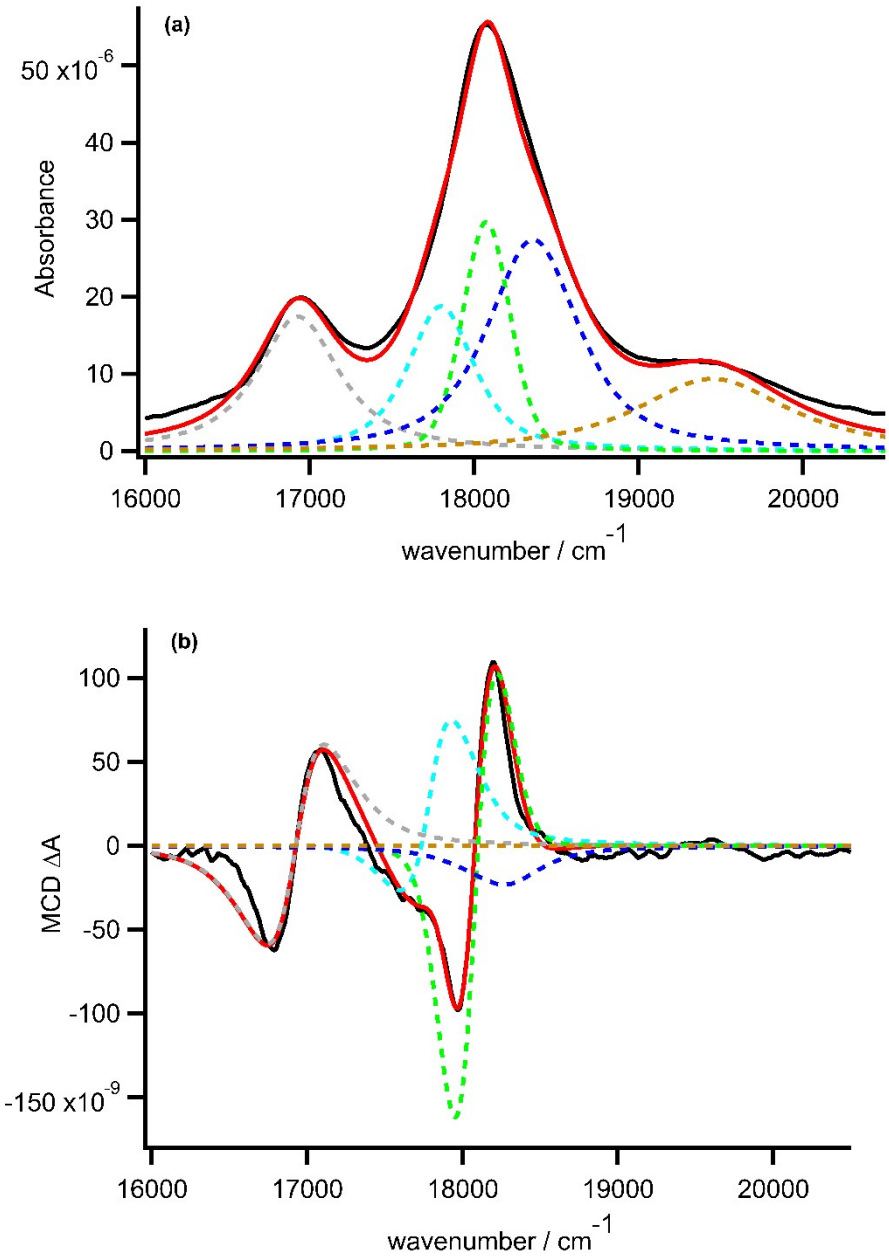

Figure S8. Band deconvolution of absorption (**a**) and MCD (**b**) of Q(0,0) and Q(1,0) bands spectra [Y(TPP)(12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

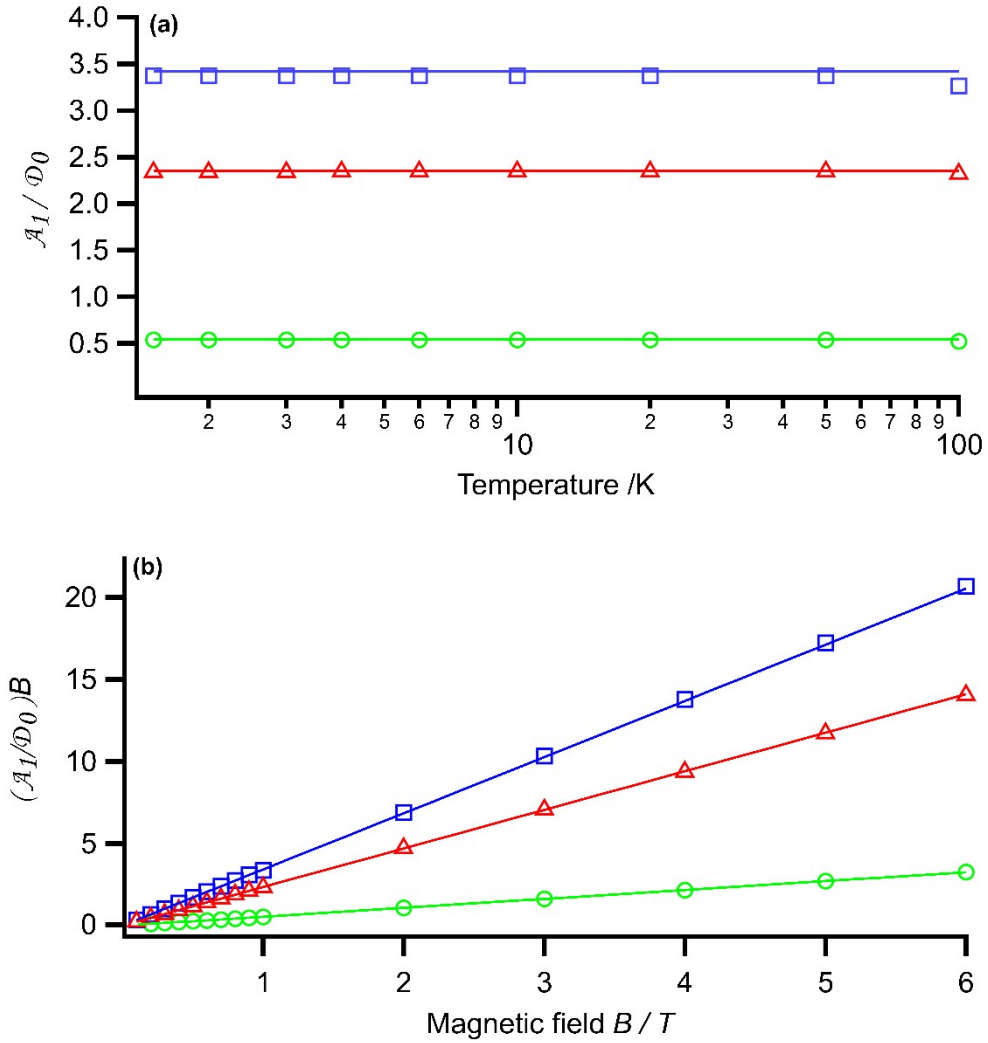

Figure S9. Experimental values (squares, triangles, and circles) and calculated value (straight line) of A_1/D_0 of [Y(TPP)(12C4)]Cl for B(0,0) in green, Q(1,0) in red, and Q(0,0) in blue under 1 T of magnetic field with varied temperature (a) and under varied magnetic field.

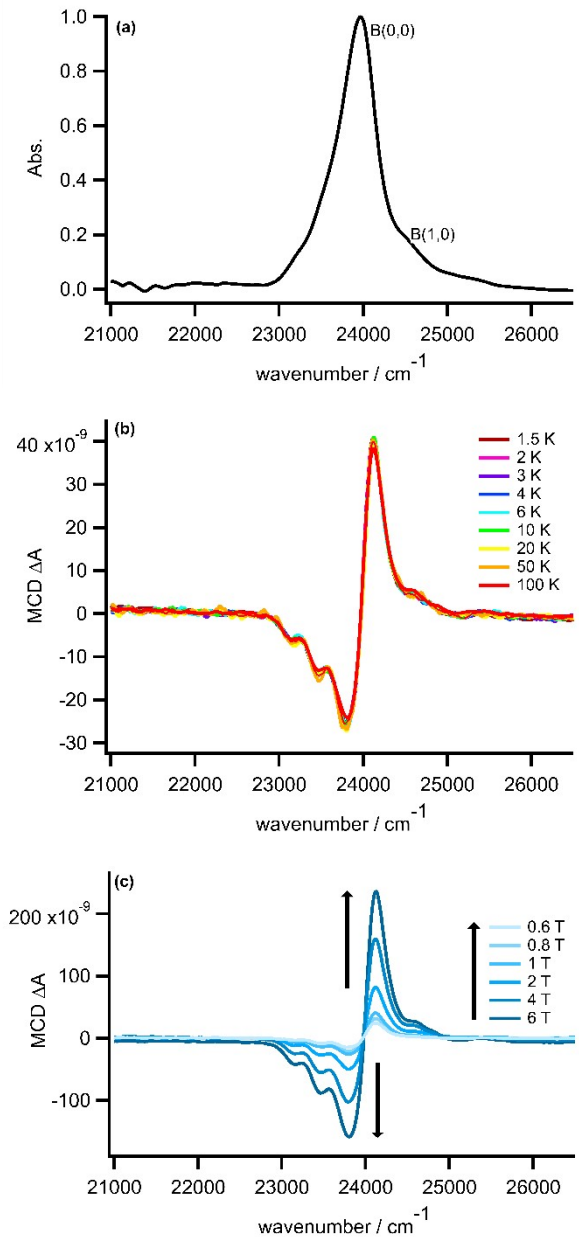

Figure S10. (a) Absorption, **(b)** temperature-dependent MCD spectra measured at temperatures of 1.5-100 K under a magnetic field of 1 T, and **(c)** magnetic fielddependent MCD spectra measured at temperatures of 1.5 K of B band in [Y(TPP) (aza12C4)]Cl in PMMA film.

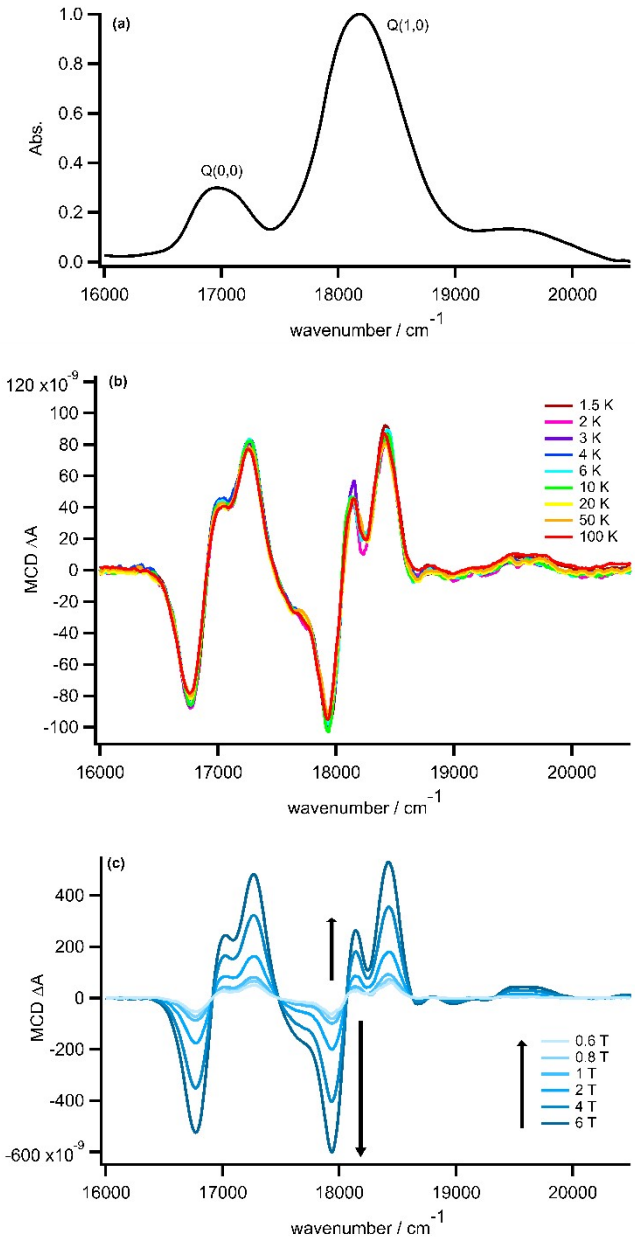

Figure S11 (a) Absorption, **(b)** temperature-dependent MCD spectra measured at temperatures of 1.5-100 K under a magnetic field of 1 T, and **(c)** magnetic field-dependent MCD spectra measured at temperatures of 1.5 K of Q band in [Y(TPP) (aza12C4)]Cl in PMMA film.

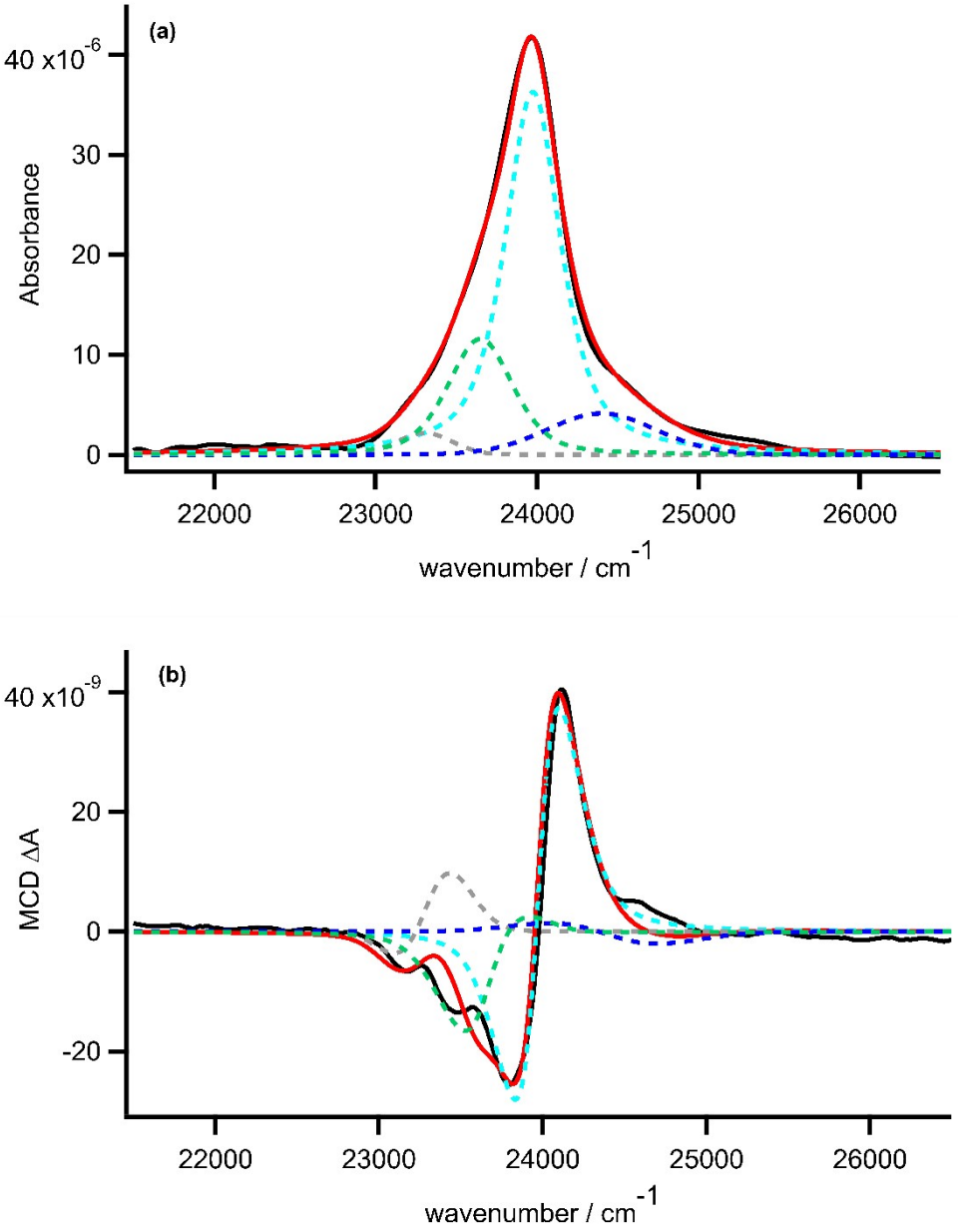

Figure S12. Band deconvolution of absorption (**a**) and MCD (**b**) of B(0,0) band spectra [Y(TPP)(aza12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

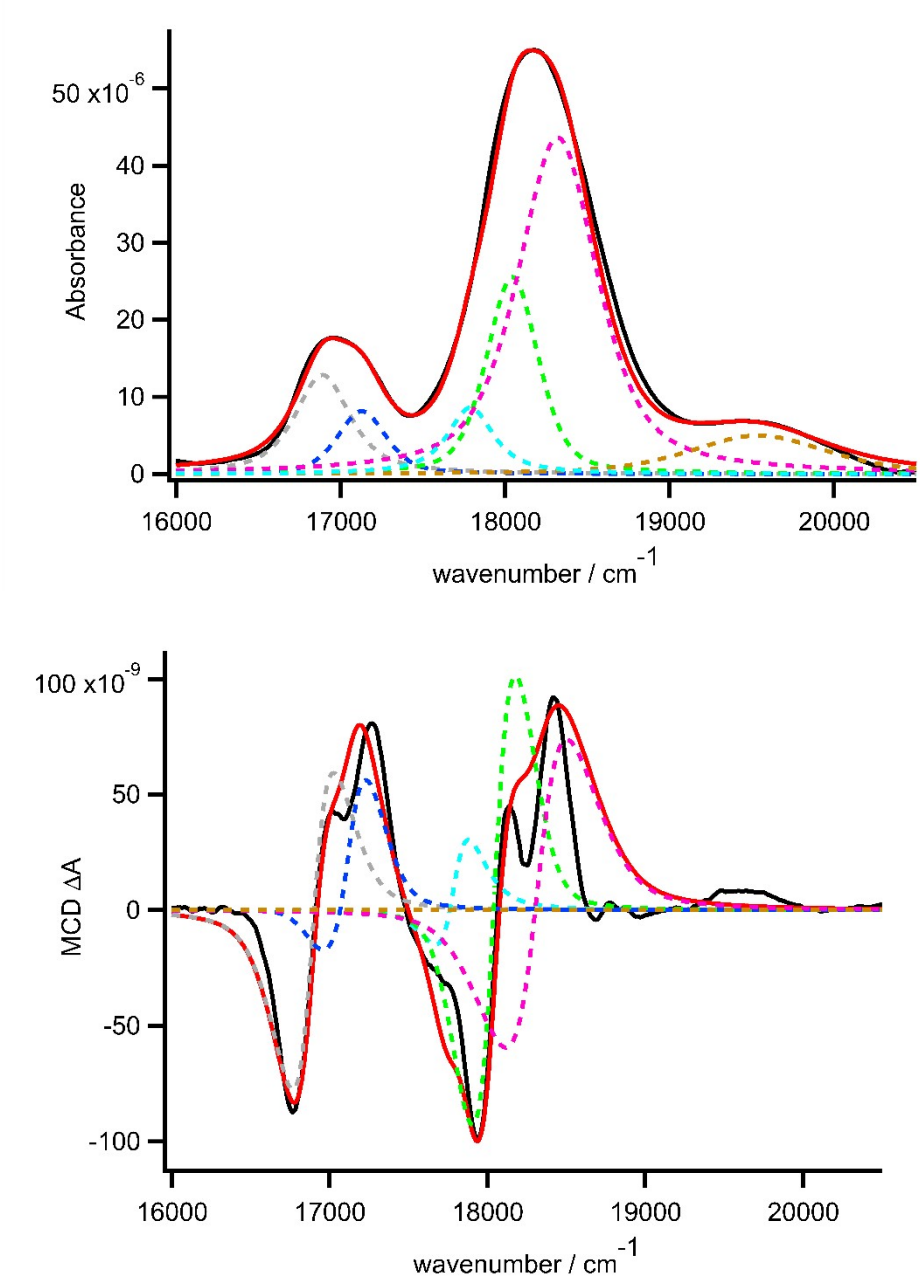

Figure S13. Band deconvolution of absorption (**a**) and MCD (**b**) of Q(0,0) and Q(1,0) bands spectra [Y(TPP)(aza12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

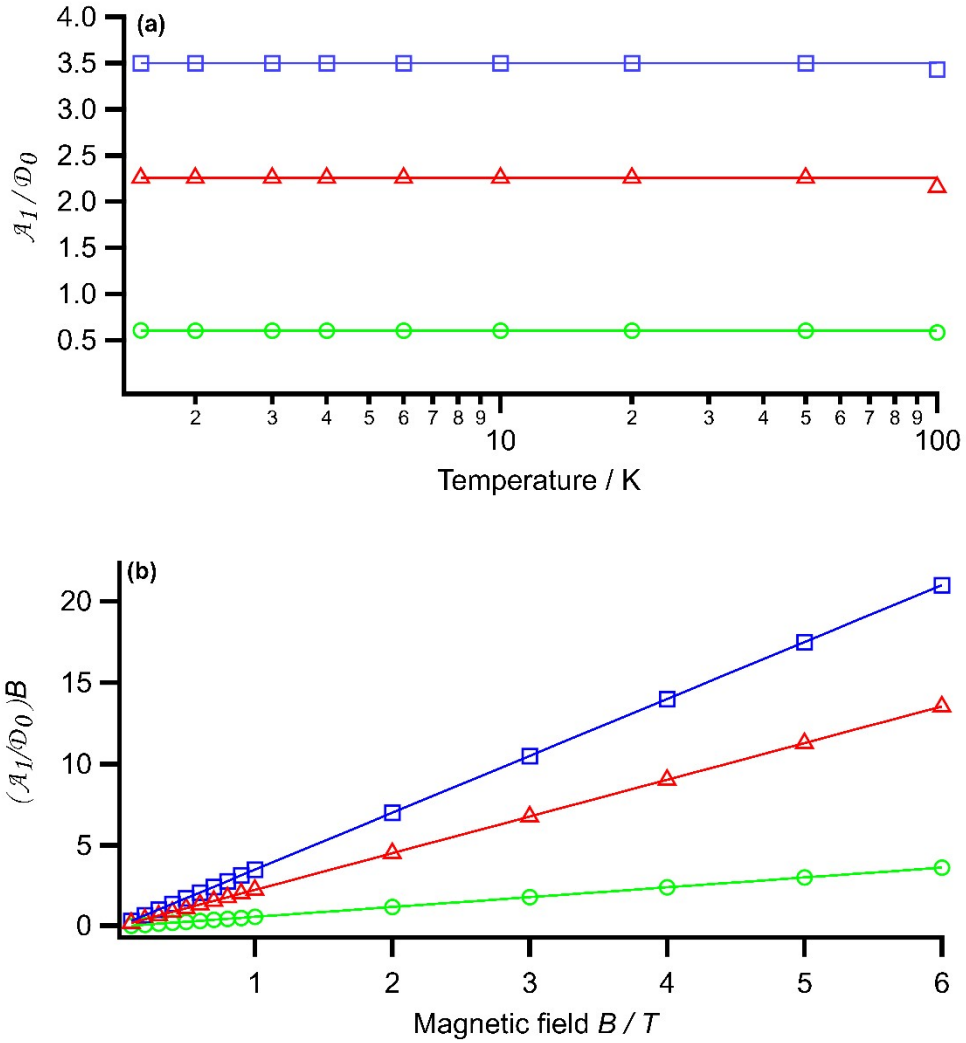

Figure S14. Experimental values (squares, triangles, and circles) and calculated value (straight line) of A_1/D_0 of [Y(TPP)(aza12C4)]Cl for B(0,0) in green, Q(1,0) in red, and Q(0,0) in blue under 1 T of magnetic field with varied temperature **(a)** and under varied magnetic field at 1.5 K **(b)**.

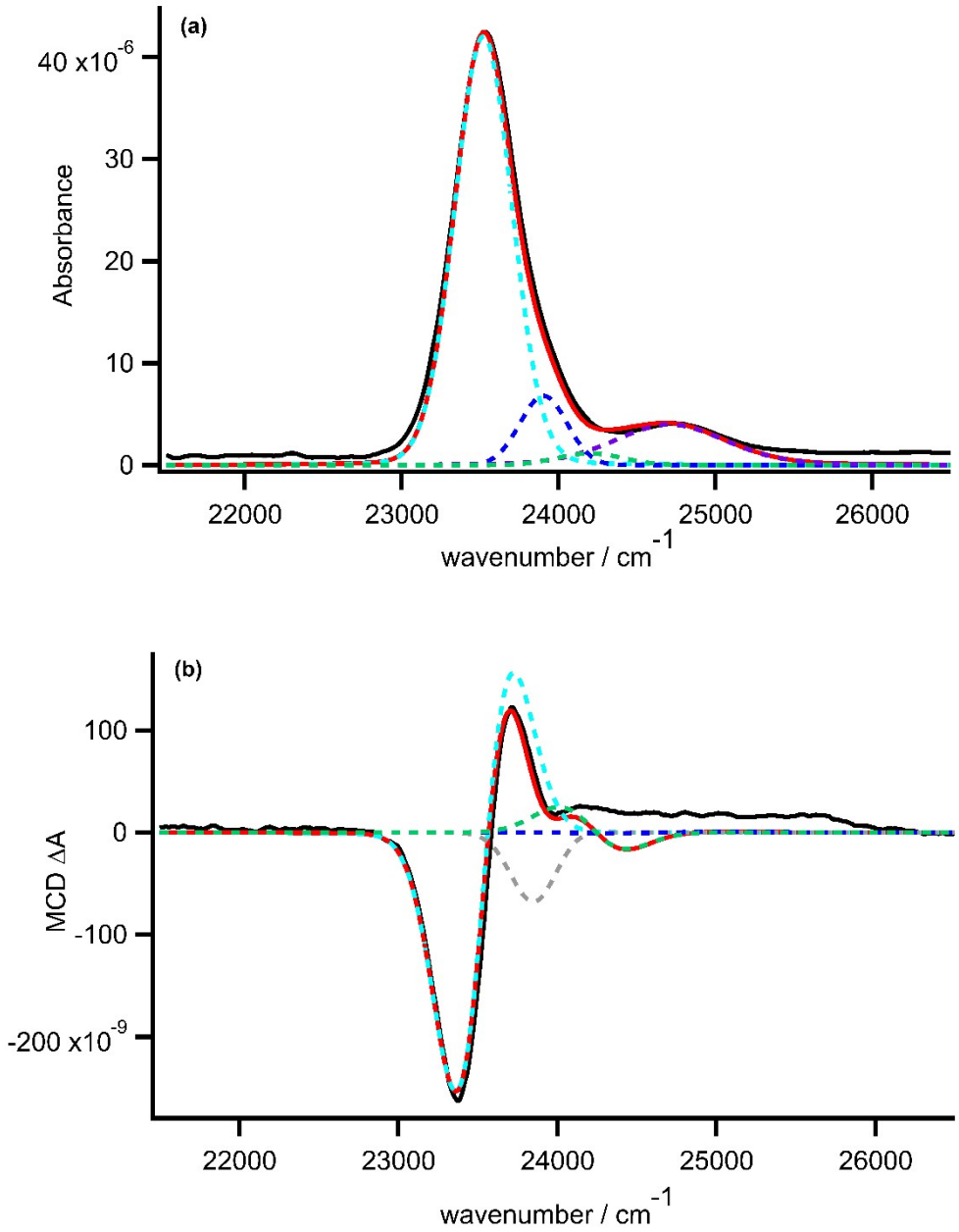

Figure S15. Band deconvolution of absorption (**a**) and MCD (**b**) of B(0,0) band spectra [Tb(TPP)(12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

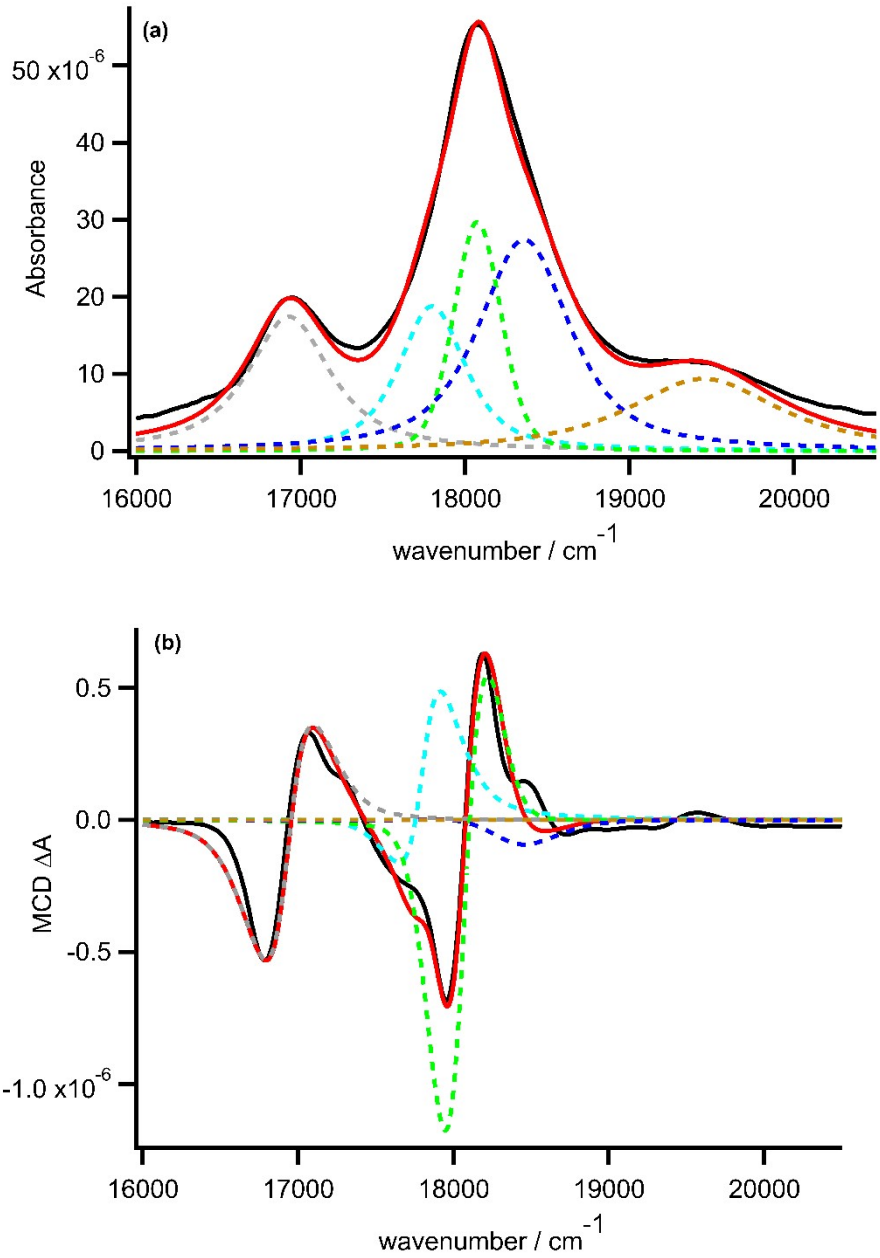

Figure S16. Band deconvolution of absorption (**a**) and MCD (**b**) of Q(0,0) and Q(1,0) bands spectra [Tb(TPP)(12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

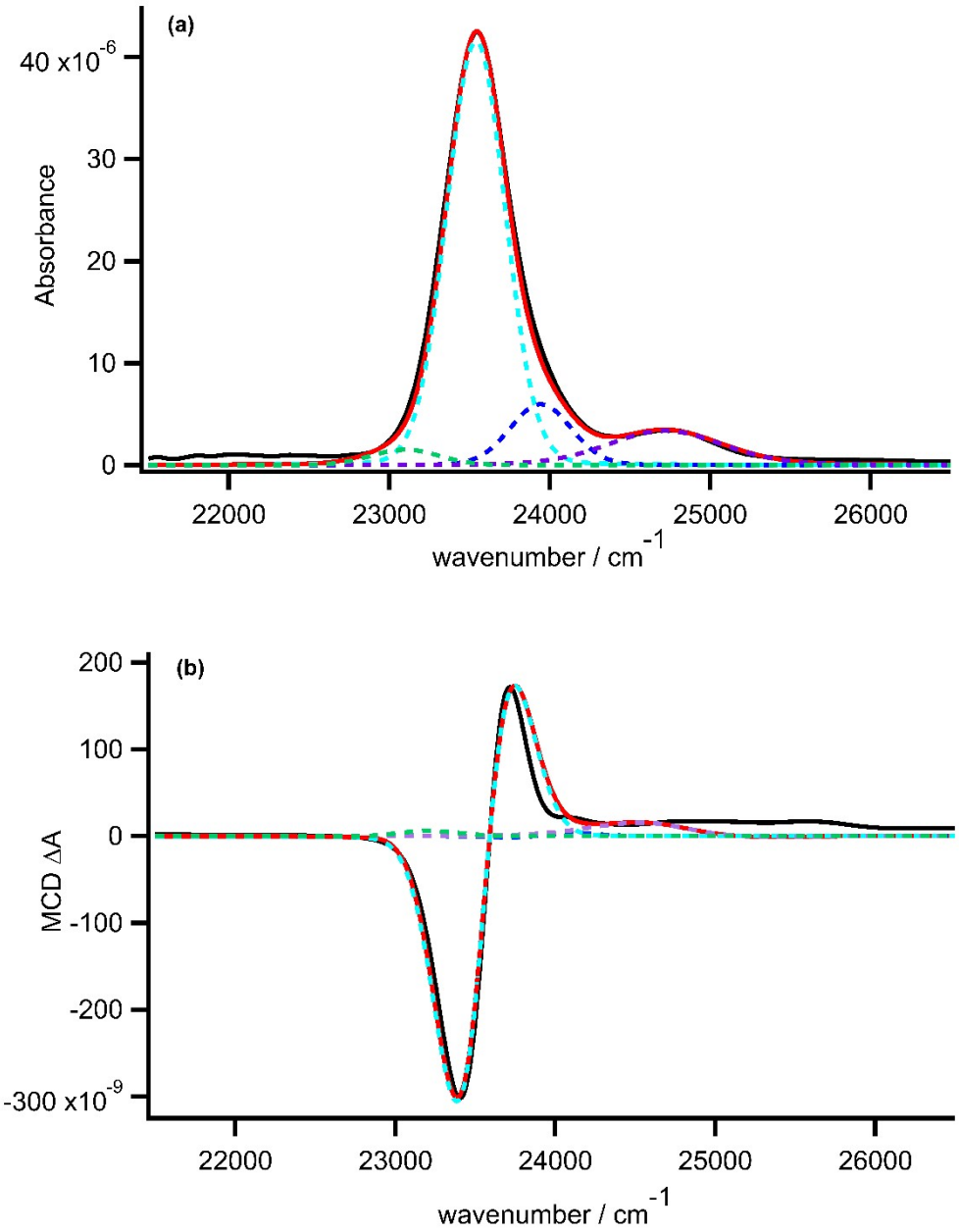

Figure S17. Band deconvolution of absorption (**a**) and MCD (**b**) of B(0,0) band spectra [Tb(TPP)(aza12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

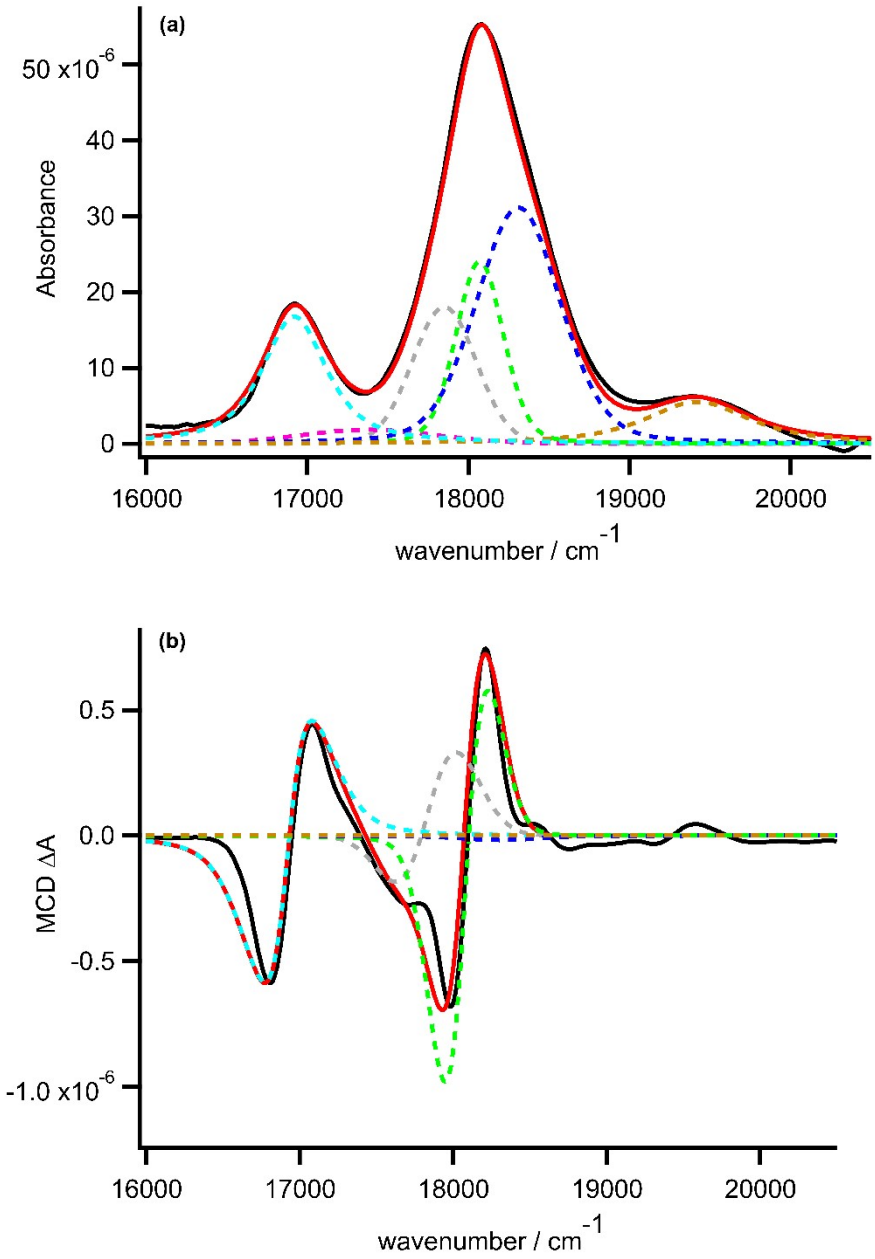

Figure S18. Band deconvolution of absorption (**a**) and MCD (**b**) of Q(0,0) and Q(1,0) bands spectra [Tb(TPP)(aza12C4)]Cl at 1.5 K and 1 T. Experimental spectra is shown in black while simulated band is in red color. The components that give the simulated band are in dashed lines.

Table S1. Parameters of B and Q bands determined by the band deconvolution of absorption and MCD spectra of [Y(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 $(cm^{-1})^{\xi}$		16930	17800	18075	18360	19450	23522	23905	24200	24700
Γ $(cm^{-1})^{\xi}$		600	480	340	660	1100	431	390	500	910
η^{ξ}		0.89	0.76	0.31	0.78	0.89	0.08	0.00	0.50	0.30
D_0		0.62	0.51	0.47	1.03	0.62	21.56	4.02	0.26	2.78
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	3.26451	2.06186	2.32179	0.1946	0.00000	0.52240	0.05827	-3.90625	0.35997
	B_0/D_0	0.00048	0.00434	-0.00300	-0.00165	0.00000	-0.00037	0.00099	0.02148	0.00000
1.5	A_1/D_0	3.41342	2.06186	2.33863	0.19461	0.00000	0.54039	0.54039	-3.90625	0.35997
	B_0/D_0	0.00016	0.00389	-0.00383	-0.00097	0.00000	-0.00045	-0.00045	0.02148	0.00000
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	3.41342	2.06186	2.33863	0.19461	0.00000	0.54039	0.54039	-3.90625	0.35997
	B_0/D_0	0.00016	0.00389	-0.00383	-0.00097	0.00000	-0.00045	-0.00045	0.02148	0.00000
2	A_1/D_0	3.35761	2.06186	2.35734	0.19461	0.00000	0.543323	0.05827	-7.8125	0.28797
	B_0/D_0	0.00024	0.00437	-0.00321	0.00000	0.00000	-0.00037	0.00049	0.01738	0.00000
3	A_1/D_0	3.35761	2.06186	2.06186	0.19461	0.00000	0.54332	0.05827	-3.90625	0.43196
	B_0/D_0	0.00024	0.00437	0.00437	0.00000	0.00000	-0.00037	0.00074	0.02519	0.00000
4	A_1/D_0	3.35761	2.06186	2.34284	0.19461	0.00000	0.54332	0.05827	-3.90625	0.35997
	B_0/D_0	0.00080	0.00437	-0.00301	0.00000	0.00000	-0.00037	0.00074	0.02519	0.00000
5	A_1/D_0	3.35761	2.06186	2.34284	0.19461	0.00000	0.54332	0.05827	-3.90625	0.35997
	B_0/D_0	0.00080	0.00437	-0.00301	0.00000	0.00000	-0.00037	0.00099	0.02556	0.00000
6	A_1/D_0	3.35762	2.06186	2.34284	0.19461	0.00000	0.54332	0.05827	-3.90625	0.35997
	B_0/D_0	0.00080	0.00433	-0.00301	0.00000	0.00000	-0.00037	0.00099	0.02148	0.00000

Table S2. Parameters of B and Q bands determined by the band deconvolution of absorption and MCD spectra of [Y(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 $(cm^{-1})^{\xi}$		16890	17130	17790	18045	18320	19540	23305	23650	23975	24400
Γ $(cm^{-1})^{\xi}$		400	350	335	370	575	990	400	477	410	800
η^{ξ}		0.79	0.55	0.89	0.51	0.71	0.60	0.10	0.50	0.78	0.13
D_0		0.29	0.15	0.17	0.48	1.38	0.26	1.05	7.64	23.02	4.00
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	3.43126	2.06379	1.43374	2.15542	1.44822	0.00000	1.09227	0.55465	0.58564	-0.50000
	B_0/D_0	-0.00259	0.00884	0.00584	0.00000	0.00058	0.00000	0.00287	-0.00200	0.00037	-0.00025
1.5	A_1/D_0	3.49975	2.41429	1.43374	2.15542	1.43374	0.00000	1.76561	0.55465	0.60677	-0.50000
	B_0/D_0	-0.00293	0.00816	0.00000	0.00055	0.00066	0.00000	0.00494	-0.00200	0.00038	-0.00025
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	3.49975	2.41429	1.43374	2.15542	1.43374	0.00000	1.76561	0.55465	0.60677	-0.50000
	B_0/D_0	-0.00293	0.00816	0.00000	0.00055	0.00066	0.00000	0.00494	-0.00200	0.00038	-0.00025
2	A_1/D_0	3.49975	2.41429	1.43374	2.15542	1.43374	0.00000	1.43085	0.55465	0.60465	-0.50000
	B_0/D_0	-0.00293	0.00816	0.00000	0.00055	0.00066	0.00000	0.00430	-0.00200	0.00048	-0.00025
3	A_1/D_0	3.49975	2.41429	1.43374	2.15542	1.43374	0.00000	1.44424	0.55465	0.60465	-0.50000
	B_0/D_0	-0.00201	0.00816	0.00000	0.00055	0.00066	0.00000	0.00316	-0.00200	0.00036	-0.00025
4	A_1/D_0	3.49975	2.41429	1.43374	2.15542	1.43374	0.00000	1.20513	0.55465	0.60465	-0.50000
	B_0/D_0	-0.00201	0.00816	0.00000	0.00055	0.00066	0.00000	0.00287	-0.00200	0.00041	-0.00025
5	A_1/D_0	3.49975	2.41429	1.43374	2.15542	1.43374	0.00000	1.49742	0.55465	0.60465	-0.50000
	B_0/D_0	-0.00201	0.00748	0.00000	0.00055	0.00066	0.00000	0.00434	-0.00200	0.00043	-0.00025
6	A_1/D_0	3.49975	2.41429	2.15542	1.43374	1.43374	0.00000	1.28739	0.55465	0.60465	-0.50000
	B_0/D_0	-0.00201	0.00748	0.00031	0.00000	0.00066	0.00000	0.00191	-0.00200	0.00037	-0.00025

Table S3. Parameters of B and Q bands determined by the band deconvolution of absorption and MCD spectra of [Tb(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 $(cm^{-1})^{\xi}$		16935	17810	18060	18330	19450	23522	23905	24200	24710
Γ $(cm^{-1})^{\xi}$		463	410	340	580	700	431	353	500	840
η^{ξ}		0.78	0.86	0.32	0.41	0.90	0.08	0.00	0.00	0.3
D_0		0.49	0.39	0.57	0.95	0.20	24.51	3.15	0.76	4.88
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	4.17493	4.12796	3.30086	0.22681	0.00000	0.66040	0.31723	-3.07275	0.20501
	B_0/D_0	0.00000	0.01565	-0.00763	-0.00311	0.00000	0.00075	-0.00317	0.01568	0.00000
1.5	A_1/D_0	19.33305	14.25014	13.23885	-1.0543	0.00000	3.14332	1.26895	-13.22751	0.20501
	B_0/D_0	-0.01511	0.02982	-0.03296	-0.00297	0.00000	-0.00403	-0.01972	0.01323	0.00000
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	19.33305	14.25014	13.23885	-1.0543	0.00000	3.14332	1.26895	-13.22751	0.20501
	B_0/D_0	-0.01511	0.02982	-0.03296	-0.00297	0.00000	-0.00403	-0.01972	0.01323	0.00000
2	A_1/D_0	12.33618	9.20003	8.52986	-1.05429	0.00000	1.96002	-0.11103	1.32275	-0.41002
	B_0/D_0	-0.00832	0.02983	-0.02419	-0.00297	0.00000	-0.00235	-0.00415	0.02622	0.00000
3	A_1/D_0	9.134167	7.89442	6.85377	-1.05429	0.00000	1.44031	-0.11103	-1.32275	-0.41002
	B_0/D_0	-0.00491	0.02858	-0.01995	-0.00297	0.00000	-0.00162	-0.00101	0.02411	0.00000
4	A_1/D_0	7.78777	5.36936	5.59515	-1.05429	0.00000	1.23627	-0.11103	-2.64550	-0.41002
	B_0/D_0	-0.00457	0.01848	-0.01427	-0.00297	0.00000	-0.00130	-0.00101	0.01719	0.00000
5	A_1/D_0	7.09438	5.36936	5.06911	-1.05429	0.00000	1.11384	-0.11103	-2.64550	-0.41002
	B_0/D_0	-0.00375	0.01776	-0.01469	-0.00125	0.00000	-0.00095	-0.00101	0.01719	0.00000
6	A_1/D_0	6.48245	5.36936	4.54305	-1.05429	0.00000	1.03223	-0.11103	-1.32275	-0.41002
	B_0/D_0	-0.00242	0.01776	-0.01469	-0.00125	0.00000	-0.00081	-0.00101	0.01362	0.00000

Table S4. Parameters of B and Q bands determined by the band deconvolution of absorption and MCD spectra of [Tb(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 $(cm^{-1})^{\xi}$		16920	17380	17850	18070	18310	19420	23100	23542	23945	24720
Γ $(cm^{-1})^{\xi}$		474	1000	465	345	614	770	500	430	450	840
η^{ξ}		0.78	0.10	0.03	0.25	0.28	0.83	0.00	0.08	0.10	0.27
D_0		0.49	0.09	0.39	0.42	0.98	0.27	1.00	24.15	3.65	4.08
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	4.58032	0.00000	4.51085	4.21337	0.00000	0.00000	0.50000	0.62048	0.09404	0.02452
	B_0/D_0	0.00238	0.00000	0.01693	-0.01639	-0.00119	0.00000	-0.00400	-0.00034	0.50000	0.00000
1.5	A_1/D_0	24.18027	0.00000	9.78821	17.10965	0.00000	0.00000	1.00000	3.68446	0.27375	-2.35715
	B_0/D_0	-0.01136	0.00000	0.01440	-0.02833	-0.00119	0.00000	0.00700	-0.00556	1.00000	0.00785
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	24.18027	0.00000	9.78821	17.10965	0.00000	0.00000	1.00000	3.68446	0.27375	-2.35715
	B_0/D_0	-0.01136	0.00000	0.01440	-0.02833	-0.00119	0.00000	0.00700	-0.00556	1.00000	0.00785
2	A_1/D_0	14.59789	0.00000	7.26315	10.99485	0.00000	0.00000	0.00000	2.20465	0.18459	-0.39531
	B_0/D_0	0.00472	0.00000	0.01440	-0.01888	-0.00184	0.00000	-0.00600	-0.00271	0.00000	0.00245
3	A_1/D_0	10.93451	0.00000	5.77642	8.65523	0.00000	0.00000	0.00000	1.66635	0.20345	-0.39531
	B_0/D_0	-0.00228	0.00000	0.01440	-0.01725	-0.00184	0.00000	-0.00600	-0.00193	0.00000	0.00245
4	A_1/D_0	9.19401	0.00000	5.37525	7.48263	0.00000	0.00000	0.00000	1.40454	0.21899	-0.39531
	B_0/D_0	-0.00061	0.00000	0.01440	-0.01661	-0.00119	0.00000	-0.00600	-0.00151	0.00000	0.00245
5	A_1/D_0	8.12400	0.00000	5.08262	6.84545	0.00000	0.00000	0.00000	1.25295	0.16425	-0.39531
	B_0/D_0	0.00069	0.00000	0.01440	-0.01661	-0.00119	0.00000	-0.00600	-0.00118	0.00000	0.00245
6	A_1/D_0	7.42056	0.00000	4.83012	6.41835	0.00000	0.00000	0.00000	1.15609	0.13687	-0.39531
	B_0/D_0	0.00131	0.00000	0.01440	-0.01661	-0.00119	0.00000	-0.00600	-0.00103	0.00000	0.00245

Computational Chemistry Calculation

Table S5. The description of Basis Sets for calculation of the [Ln(TPP)L]Cl (Ln = Y and Tb; L = (12C4 and aza12C4) complexes.

Basis Set 1	*Basis Set 2*
Tb.ANO-RCC...8s7p5d3f2g1h	Tb.ANO-RCC...7s6p4d2f1g
Y. ANO-RCC...7s6p4d2f1g	Y. ANO-RCC...6s5p3d1f
C.ANO-RCC...2s1p	C.ANO-RCC...2s1p
N.ANO-RCC...2s1p	N.ANO-RCC...2s1p
O.ANO-RCC...2s1p	O.ANO-RCC...2s1p
H.ANO-RCC...1s	H.ANO-RCC...1s

Table S6. Dipole transition strengths for $[Y(TPP)(12C4)]^+$ obtained from RASSCF/RASSI/single_aniso calculations.

Basis Set 1						
From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	2	2.79×10^{-4}	2.01×10^{2}	1.26×10^{5}	2.11×10^{2}	1.26×10^{5}
1	3	2.50×10^{-4}	1.12×10^{5}	9.88×10^{1}	6.73×10^{2}	1.13×10^{5}
1	4	5.45	3.76×10^{8}	7.78×10^{9}	5.35×10^{-1}	8.16×10^{9}
1	5	5.45	7.80×10^{9}	3.77×10^{8}	4.53×10^{2}	8.18×10^{9}
2	4	4.91×10^{-4}	1.02×10^{5}	5.34×10^{2}	4.71×10^{4}	1.49×10^{5}
2	5	4.69×10^{-4}	1.21×10^{2}	1.26×10^{5}	1.73×10^{4}	1.43×10^{5}
3	4	5.14×10^{-4}	7.06	1.39×10^{5}	1.72×10^{4}	1.56×10^{5}
3	5	4.92×10^{-4}	1.04×10^{5}	3.53×10^{1}	4.64×10^{4}	1.50×10^{5}
Basis Set 2						
From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	2	1.77×104	1.02×10^{4}	7.18×10^{4}	3.55×10^{2}	8.24×10^{4}
1	3	1.59×104	6.64×10^{4}	7.74×10^{3}	1.77	7.41×10^{4}
1	4	5.49	5.52×10^{9}	2.83×10^{9}	7.83×10^{-1}	8.35×10^{9}
1	5	5.49	2.83×10^{9}	5.53×10^{9}	2.04×10^{2}	8.36×10^{9}
2	4	1.81×10-^{4}	1.17×10^{4}	4.23×10^{4}	1.05×10^{3}	5.50×10^{4}
2	5	4.00×10-^{4}	4.94×10^{4}	1.55×10^{4}	5.66×10^{4}	1.21×10^{5}
3	4	4.17×10^{-4}	5.17×10^{4}	1.83×10^{4}	5.65×10^{4}	1.26×10^{5}
3	5	1.73×10^{-4}	1.27×10^{4}	3.88×10^{4}	1.04×10^{3}	5.25×10^{4}

Table S7. Low-Lying Spin Orbit of $[Y(TPP)(12C4)]^+$ obtained from RASSCF/RASSI/single_aniso calculations.

Basis Set 1						
S.O states	Energy (cm^{-1})	g_z	g_x	g_y	L_z	S_z
1	0.00	-	-	-	-	
2	26049.06005	8.14	0.00	0.00	4.07	0.00
3	26051.51537					
4	47392.89823	0.36	0.00	0.00	0.18	0.00
5	47431.70499					
Basis Set 2						
S.O states	Energy (cm^{-1})	g_z	g_x	g_y	L_z	S_z
1	0.00	-	-	-	-	-
2	26431.10	8.11	0.00	0.00	4.05	0.00
3	26431.65					
4	47760.09	0.33	0.00	0.00	0.16	0.00
5	47777.50					

Table S8. Dipole transition strengths for $[Y(TPP)(aza12C4)]^+$ obtained from RASSCF/RASSI/single_aniso calculations.

Basis Set 1						
From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	2	2.24×10^{-3}	4.20×10^{5}	5.91×10^{5}	3.43	1.01×10^{6}
1	3	7.59×10^{-4}	8.03×10^{1}	3.44×10^{5}	4.11	3.44×10^{5}
1	4	5.44	4.78×10^{9}	3.28×10^{9}	4.05×10^{4}	8.07×10^{9}
1	5	5.44	3.30×10^{9}	4.79×10^{9}	1.61×10^{3}	8.09×10^{9}
2	4	4.61×10^{-3}	1.07×10^{6}	1.87×10^{5}	1.18×10^{5}	1.37×10^{6}
2	5	3.12×10^{-3}	7.18×10^{5}	2.07×10^{5}	8.66×10^{3}	9.34×10^{5}
3	4	1.07×10^{-3}	6.46×10^{4}	2.37×10^{5}	1.47×10^{4}	3.17×10^{5}
3	5	1.58×10^{-3}	5.34×10^{4}	3.81×10^{5}	3.74×10^{4}	4.72×10^{5}
Basis Set 2						
From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	2	1.95×10^{-3}	1.33×10^{5}	7.80×10^{5}	2.50×10^{3}	9.16×10^{5}
1	3	5.68×10^{-4}	1.83×10^{4}	2.49×10^{5}	5.44×10^{2}	2.67×10^{5}
1	4	5.42	1.84×10^{9}	6.33×10^{9}	$2.68E\times10^{4}$	8.17×10^{9}
1	5	5.44	6.40×10^{9}	1.85×10^{9}	5.89×10^{3}	8.26×10^{9}
2	4	2.53×10^{-3}	6.50×10^{5}	1.69×10^{3}	9.30×10^{4}	7.45×10^{5}
2	5	1.09×10^{-2}	3.21×10^{6}	1.24×10^{4}	3.37×10^{4}	3.26×10^{6}
3	4	1.74×10^{-3}	3.60×10^{5}	1.37×10^{5}	1.36×10^{4}	5.11×10^{5}
3	5	3.58×10^{-3}	3.53×10^{4}	1.01×10^{6}	2.53×10^{4}	1.07×10^{6}
4	5	9.92×10^{-5}	7.58×10^{-1}	1.65	3.97×10^{-8}	2.41

Table S9. Low-Lying Spin Orbit of $[Y(TPP)(aza12C4)]^+$ obtained from RASSCF/RASSI/single_aniso calculations

Basis Set 1						
S.O states	Energy (cm^{-1})	g_z	g_x	g_y	L_z	S_z
1	0.00	-	-	-	-	-
2	26030.76	8.07	0.00	0.00	4.03	0.00
3	26063.59					
4	47151.07	0.37	0.00	0.00	0.19	0.00
5	47212.79					
Basis Set 2						
S.O states	Energy (cm^{-1})	g_z	g_x	g_y	L_z	S_z
1	0.00	-	-	-	-	-
2	26525.77	8.03	0.00	0.00	4.01	0.00
3	26566.83					
4	47524.82	0.34	0.00	0.00	0.17	0.00
5	47715.52					

Table S10. Composition of wave functions for $[Tb(TPP)(12C4)]^+$ as extracted from RASSCF/RASSI/Single_Aniso calculations with basis set 1.

M_J	**Wave Functions and Energies**					
	1		**2**		**3**	
	0.000 cm^{-1}		0.179 cm^{-1}		120.229 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.391338-0.587270i	0.498	0.391800-0.587962i	0.499	0.000000	0.000
-5	0.000000	0.000	0.000000	0.000	-0.282917+0.402093i	0.242
-4	0.000000	0.000	0.000000	0.000	0.000000	0.000
-3	0.000000	0.000	0.000000	0.000	0.171332+0.176008i	0.060
-2	-0.039904-0.019410i	0.002	-0.025332-0.012311i	0.001	0.000000	0.000
-1	0.000000	0.000	0.000000	0.000	0.413028+0.165389i	0.198
0	0.000000	0.000	0.000000	0.000	0.000000	0.000
1	0.000000	0.000	0.000000	0.000	0.208420-0.393074i	0.198
2	-0.005976+0.043970i	0.002	0.003802-0.027907i	0.001	0.000000	0.000
3	0.000000	0.000	0.000000	0.000	0.017071-0.245035i	0.060
4	0.000000	0.000	0.000000	0.000	0.000000	0.000
5	0.000000	0.000	0.000000	0.000	-0.475719-0.124147i	0.242
6	0.705713	0.498	-0.706546	0.499	0.000000	0.000
M_J	**4**		**5**		**6**	
	120.229 cm^{-1}		127.393 cm^{-1}		136.541 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.000000	0.000	0.000000	0.000	0.024656-0.036894i	0.002
-5	0.373254-0.320004i	0.242	0.000000	0.000	0.000000	0.000
-4	0.000000	0.000	0.079033-0.405279i	0.170	0.000000	0.000
-3	0.122691+0.212791i	0.060	0.000000	0.000	0.000000	0.000
-2	0.000000	0.000	0.000000	0.000	0.634192+0.309567i	0.498
-1	-0.359555-0.262042i	0.198	0.000000	0.000	0.000000	0.000
0	0.000001	0.000	-0.808278+0.075450i	0.659	0.000000	0.000
1	0.298831-0.329615i	0.198	0.000000	0.000	0.000000	0.000
2	0.000000	0.000	0.000000	0.000	0.095004-0.699289i	0.498
3	-0.076910+0.233277i	0.060	0.000000	0.000	0.000000	0.000
4	0.000000	0.000	0.152676+0.383650i	0.170	0.000000	0.000

5	-0.430474-0.237514i	0.242	0.000000	0.000	0.000000	0.000
6	0.000000	0.000	0.000000	0.000	0.044374	0.002
M_J	**7**		**8**		**9**	
	154.392 cm^{-1}		154.392 cm^{-1}		194.587 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.000000	0.000	0.000000	0.000	0.000000	0.000
-5	-0.446607-0.219440i	0.248	0.491260+0.079224i	0.248	0.000000	0.000
-4	0.000000	0.000	0.000000	0.000	-0.614274+0.350239i	0.500
-3	0.178587+0.310817i	0.129	0.261683+0.244994i	0.129	0.000000	0.000
-2	0.000000	0.000	0.000000	0.000	0.000000	0.000
-1	0.078387-0.343137i	0.124	0.025399+0.351059i	0.124	0.000000	0.000
0	0.000000	0.000	0.000000	0.000	0.000151-0.000157i	0.000
1	0.236692-0.260508i	0.124	0.150151-0.318343i	0.124	0.000000	0.000
2	0.000000	0.000	0.000000	0.000	0.000000	0.000
3	-0.357109+0.031205i	0.129	0.332368-0.134285i	0.129	0.000000	0.000
4	0.000000	0.000	0.000000	0.000	-0.326941+0.626984i	0.500
5	0.435391+0.240929i	0.248	0.486818+0.103054i	0.248	0.000000	0.000
6	0.000000	0.000	0.000000	0.000	0.000000	0.000
M_J	**10**		**11**		**12**	
	231.000 cm^{-1}		232.305 cm^{-1}		232.470 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	-0.015671+0.023403i	0.001	0.000000	0.000	0.000000	0.000
-5	0.000001i	0.000	0.000006+0.000001i	0.000	-0.094562+0.041536i	0.011
-4	0.000002	0.000	0.561081-0.121206i	0.330	0.000028-0.000004i	0.000
-3	0.000002+0.000002i	0.000	-0.000028+0.000017i	0.000	0.556609+0.036780i	0.311
-2	-0.634799-0.310221i	0.499	0.000002+0.000001i	0.000	0.000002+0.000001i	0.000
-1	-0.000002	0.000	0.000003+0.000025i	0.000	-0.254357-0.336852i	0.178
0	0.000001+0.000001i	0.000	0.279385+0.512775i	0.341	0.000012+0.000026i	0.000
1	-0.000001+0.000002i	0.000	-0.000019-0.000016i	0.000	0.102615+0.409435i	0.178
2	0.095436-0.700071i	0.499	0.000002i	0.000	-0.000001+0.000003i	0.000
3	-0.000001-0.000003i	0.000	-0.000030+0.000014i	0.000	0.320696-0.456421i	0.311
4	-0.000001+0.000001i	0.000	-0.406054+0.405737i	0.330	-0.000021+0.000019i	0.000
5	-0.000001	0.000	0.000003-0.000005i	0.000	-0.091685+0.047552i	0.011
6	0.028165	0.001	0.000000	0.000	0.000000	0.000

M_J	**13**	
	232.470 cm^{-1}	
	c	|c|
-6	0.000000	0.000
-5	-0.048733-0.091062i	0.011
-4	0.000018-0.000005i	0.000
-3	-0.006429-0.557786i	0.311
-2	-0.000002-0.000001i	0.000
-1	0.316145-0.279676i	0.178
0	0.000009+0.000016i	0.000
1	0.400260-0.134010i	0.178
2	0.000000-0.000003i	0.000
3	0.479883+0.284391i	0.311
4	-0.000013+0.000013i	0.000
5	0.054508+0.087727i	0.011
6	0.000000	0.000

Table S11. Composition of wave functions for $[Tb(TPP)(12C4)]^+$ as extracted from RASSCF/RASSI/single_Aniso calculations with basis set 2.

M_J	**Wave Functions and Energies**					
	1		**2**		**3**	
	0.000 cm^{-1}		0.105 cm^{-1}		123.232 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	-0.514067-0.484233i	0.499	-0.514415-0.484562i	0.499	0.000000	0.000
-5	0.000000	0.000	0.000000	0.000	-0.324541-0.484521i	0.340
-4	-0.000002+0.000003i	0.000	-0.000002+0.000003i	0.000	0.000000	0.000
-3	0.000000	0.000	0.000000	0.000	-0.130626+0.124459i	0.033
-2	0.029828+0.019086i	0.001	0.020241+0.012943i	0.001	0.000000	0.000
-1	0.000000	0.000	0.000000	0.000	0.275601+0.226724i	0.127
0	-0.000001i	0.000	0.000000	0.000	0.000000	0.000
1	0.000000	0.000	0.000000	0.000	0.149856-0.323887i	0.127
2	-0.034799-0.006559i	0.001	0.023608+0.004457i	0.001	0.000000	0.000
3	0.000000	0.000	0.000000	0.000	-0.171704-0.055414i	0.033
4	-0.000001+0.000004i	0.000	0.000001-0.000003i	0.000	0.000000	0.000
5	0.000000	0.000	0.000000	0.000	-0.082033+0.577372i	0.000
6	0.706220	0.499	-0.706699	0.499	0.000000	0.000
M_J	**4**		**5**		**6**	
	123.233 cm^{-1}		135.406 cm^{-1}		144.439 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.000000	0.000	-0.000001-0.000002i	0.000	-0.025741-0.024318i	0.001
-5	-0.115691-0.571583i	0.340	0.000000	0.000	0.000000	0
-4	0.000000	0.000	0.322137-0.283850i	0.184	0.000004-0.000004i	0
-3	0.168153-0.065366i	0.033	0.000000	0.000	0.000000	0
-2	0.000000	0.000	0.000001+0.000001i	0.000	-0.594292-0.381527i	0.499
-1	0.168560+0.314560i	0.127	0.000000	0.000	0.000000	0
0	0.000000	0.000	-0.380484+0.697528i	0.631	0.000001-0.000003i	0
1	-0.261857+0.242468i	0.127	0.000000	0.000	0.000000	0
2	0.000000	0.000	-0.000001-0.000001i	0.000	0.694004+0.130782i	0.499
3	-0.137677-0.116590i	0.033	0.000000	0.000	0.000000	0
4	0.000000	0.000	0.064259-0.424516i	0.184	0.000000-0.000005i	0
5	0.295623-0.502692i	0.340	0.000000	0.000	0.000000	0
6	0.000000	0.000	0.000003	0.000	0.035411	0.001
M_J	**7**		**8**		**9**	
	154.526 cm^{-1}		154.527 cm^{-1}		189.843 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.000000	0.000	0.000000	0.000	-0.000002-0.000003i	0.000
-5	-0.446607-0.219440i	0.152	-0.157096-0.356840i	0.152	0.000000	0.000
-4	0.000000	0.000	0.000000	0.000	0.524728-0.473984i	0.500
-3	0.178587+0.310817i	0.157	0.339485-0.205395i	0.157	0.000000	0.000
-2	0.000000	0.000	0.000000	0.000	-0.000009-0.000007i	0.000
-1	0.078387-0.343137i	0.191	-0.283479-0.331946i	0.191	0.000000	0.000
0	0.000000	0.000	0.000000	0.000	0.000174+0.000092i	0.000
1	0.236692-0.260508i	0.191	-0.264207+0.347482i	0.191	0.000000	0.000
2	0.000000	0.000	0.000000	0.000	-0.000011-0.000003i	0.000
3	-0.357109+0.031205i	0.157	0.350582+0.185821i	0.157	0.000000	0.000
4	0.000000	0.000	0.000000	0.000	-0.096839+0.700444i	0.500
5	0.435391+0.240929i	0.152	-0.136616+0.365171i	0.152	0.000000	0.000
6	0.000000	0.000	0.000000	0.000	-0.000004	0.000
M_J	**10**		**11**		**12**	
	223.889 cm^{-1}		226.431 cm^{-1}		226.569 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	-0.000002-0.000001i	0.000	-0.017451-0.016513i	0.001	0.000000	0.000

-5	0.000000	0.000	0.000000	0.000	0.039130+0.079806i	0.008
-4	0.356339-0.434373i	0.316	-0.000014+0.000003i	0.000	0.000000	0.000
-3	0.000000	0.000	0.000001-0.000001i	0.000	-0.531900-0.164597i	0.310
-2	0.000012i	0.000	-0.594540-0.382028i	0.499	-0.000001-0.000001i	0.000
-1	0.000000	0.000	0.000000-0.000001i	0.000	0.290454+0.312612i	0.182
0	0.201053-0.572943i	0.369	-0.000009-0.000004i	0.000	0.000000	0.000
1	0.000000	0.000	0.000001-0.000001i	0.000	-0.425475+0.032566i	0.182
2	-0.000007+0.000010i	0.000	-0.694422-0.131154i	0.499	-0.000001	0.000
3	0.000000	0.000	0.000000-0.000001i	0.000	0.502410+0.239989i	0.310
4	-0.006772-0.561793i	0.316	-0.000008-0.000012i	0.000	0.000000	0.000
5	0.000000	0.000	0.000000	0.000	-0.082894+0.032075i	0.008
6	0.000002	0.000	-0.024025	0.001	0.000000	0.000

M_J	**13**
	226.569 cm^{-1}
	c | |c|
-6	0.000000 0.000
-5	0.079900-0.038921i 0.008
-4	0.000000 0.000
-3	0.166020-0.531458i 0.310
-2	0.000001+0.000001i 0.000
-1	0.313391-0.289616i 0.182
0	0.000000 0.000
1	-0.031430-0.425563i 0.182
2	0.000001 0.000
3	0.241332-0.501766i 0.310
4	0.000000 0.000
5	-0.031842-0.082976i 0.008
6	0.000000 0.000

Table S12. Composition of wave functions for $[Tb(TPP)(aza12C4)]^+$ as extracted from RASSCF/RASSI/single_sniso calculations with basis set 1.

M_J	**Wave Functions and Energies**					
	1		**2**		**3**	
	0.000		0.058		144.860	
	c	|c|	c	|c|	c	|c|
-6	-0.312088-0.633596i	0.499	-0.312183-0.633771i	0.499	0.008789+0.002533i	0.000
-5	0.000457-0.000686i	0.000	0.000308-0.000650i	0.000	0.072676+0.615057i	0.384
-4	0.004537+0.006879i	0.000	0.004421+0.007353i	0.000	0.173034-0.073061i	0.035
-3	-0.001084-0.013776i	0.000	-0.000680-0.014575i	0.000	-0.045447-0.137244i	0.021
-2	-0.028625+0.007447i	0.001	-0.021806+0.006194i	0.001	-0.025734+0.088616i	0.009
-1	0.003366+0.003097i	0.000	0.005282+0.006674i	0.000	0.217772+0.033026i	0.049
0	0.000938-0.001507i	0.000	0.001993+0.001240i	0.000	-0.078330-0.011063i	0.006
1	0.004266+0.001651i	0.000	-0.008321-0.001789i	0.000	-0.218400-0.028579i	0.049
2	0.005968+0.028969i	0.001	-0.004079-0.022298i	0.001	-0.000184-0.092277i	0.009
3	-0.012838+0.005115i	0.000	0.013375-0.005831i	0.000	0.081680-0.119288i	0.021
4	-0.008176-0.001030i	0.000	0.008549+0.000717i	0.000	0.146030+0.118126i	0.035
5	-0.000413+0.000713i	0.000	0.000447-0.000564i	0.000	-0.240177+0.570870i	0.384
6	0.706288	0.499	-0.706487	0.499	0.009147	0.000
M_J	**4**		**5**		**6**	
	146.052		185.998		197.469	
	c	|c|	c	|c|	c	|c|
-6	-0.010150+0.000156i	0.000	-0.004075-0.018761i	0.000	0.012842-0.017796i	0.000
-5	-0.160024-0.603205i	0.389	-0.197475+0.135514i	0.057	-0.312351+0.017898i	0.098
-4	-0.186892+0.091968i	0.043	-0.302944-0.206966i	0.135	-0.149248-0.208411i	0.066

-3	0.078484+0.034551i	0.007	-0.151217+0.310714i	0.119	-0.249251+0.303205i	0.154
-2	0.054217-0.116112i	0.016	0.231572+0.022518i	0.054	0.065783+0.268707i	0.077
-1	-0.152857+0.041066i	0.025	0.149885+0.115074i	0.036	0.068623-0.313714i	0.103
0	0.001463+0.190886i	0.036	-0.278424+0.345401i	0.197	-0.030272-0.059176i	0.004
1	-0.153468-0.038718i	0.025	0.144269+0.122040i	0.036	0.294550+0.127930i	0.103
2	-0.055990-0.115268i	0.016	-0.071164-0.221514i	0.054	0.179403+0.210583i	0.077
3	0.077945-0.035750i	0.007	0.271531-0.213730i	0.119	-0.391726+0.024693i	0.154
4	0.188280+0.089093i	0.043	0.266559+0.252104i	0.135	-0.081666-0.242982i	0.066
5	-0.150760+0.605587i	0.389	0.090505-0.221741i	0.057	-0.197293+0.242815i	0.098
6	0.010151	0.000	0.019198	0.000	-0.021945	0.000

M_J	**7**		**8**		**9**	
	205.889		220.344		248.459	
	c	|c|	c	|c|	c	|c|
-6	-0.008726+0.020867i	0.001	0.000141-0.006678i	0.000	0.006655+0.006588i	0.000
-5	0.003352+0.088188i	0.008	-0.225095+0.020625i	0.051	0.026928+0.016491i	0.001
-4	-0.119592-0.212918i	0.060	0.013986-0.101504i	0.010	-0.245605+0.544567i	0.357
-3	0.136440-0.070913i	0.024	0.063885-0.295647i	0.091	-0.045976-0.009715i	0.002
-2	-0.501422-0.178348i	0.283	0.184891-0.019904i	0.035	-0.089771+0.157752i	0.033
-1	-0.174855+0.018982i	0.031	-0.063608-0.517635i	0.272	0.173628-0.276068i	0.106
0	-0.361405+0.240606i	0.189	-0.202858+0.198626i	0.081	0.012361-0.030055i	0.001
1	0.084969-0.153996i	0.031	-0.516179-0.074506i	0.272	-0.070831+0.318344i	0.106
2	-0.028899+0.531411i	0.283	0.023798-0.184430i	0.035	-0.047186+0.175265i	0.033
3	-0.118060+0.098520i	0.024	-0.296928+0.057638i	0.091	-0.039508-0.025442i	0.002
4	0.150299+0.192475i	0.060	0.101777-0.011843i	0.010	-0.208577+0.559795i	0.357
5	0.080068+0.037114i	0.008	0.025365-0.224610i	0.051	0.030739+0.007225i	0.001
6	-0.022618	0.001	0.006680	0.000	-0.009364	0.000

M_J	**10**		**11**		**12**	
	283.594		296.282		313.474	
	c	|c|	c	|c|	c	|c|
-6	-0.003714+0.003842i	0.000	-0.000082+0.009967i	0.000	-0.007327-0.010613i	0.000
-5	0.072831-0.029779i	0.006	-0.035665+0.029484i	0.002	0.005604+0.011482i	0.000
-4	0.149051+0.395465i	0.179	-0.139516-0.090369i	0.028	0.077058-0.262607i	0.075
-3	0.037510-0.050334i	0.004	0.363077-0.285618i	0.213	0.378381-0.036797i	0.145
-2	0.112929-0.152394i	0.036	-0.274324+0.126394i	0.091	0.407168+0.016067i	0.166
-1	0.158343+0.202458i	0.066	-0.245546-0.308290i	0.155	-0.149835+0.267662i	0.094
0	-0.595481+0.252560i	0.418	-0.100388-0.101217i	0.020	0.177567+0.093185i	0.040
1	0.035492+0.254562i	0.066	0.306260+0.248073i	0.155	-0.135142+0.275373i	0.094
2	0.188056+0.024738i	0.036	0.128645-0.273275i	0.091	0.244548+0.325944i	0.166
3	-0.062259-0.008019i	0.004	0.288594-0.360716i	0.213	-0.184690-0.332289i	0.145
4	-0.180709-0.382038i	0.179	-0.089218-0.140255i	0.028	-0.172330+0.212610i	0.075
5	-0.072032+0.031662i	0.006	-0.029776+0.035421i	0.002	-0.012633+0.001911i	0.000
6	-0.005344	0.000	0.009967	0.000	-0.012897	0.000

M_J	**13**	
	317.366	
	c	|c|
-6	0.000591+0.007593i	0.000
-5	0.057729+0.002612i	0.003
-4	0.112525+0.007784i	0.013
-3	0.135013+0.447698i	0.219
-2	-0.437633+0.086493i	0.199
-1	-0.131413+0.213213i	0.063
0	-0.061275-0.056695i	0.007
1	-0.202381+0.147550i	0.063
2	0.052298-0.443023i	0.199
3	-0.456819-0.099891i	0.219
4	0.016486+0.111583i	0.013

5	-0.007080-0.057353i	0.003
6	0.007616	0.000

Table S13. Composition of wave functions for $[Tb(TPP)(aza12C4)]^+$ as extracted from RASSCF/RASSI/single_aniso calculations with basis set 2.

M_J	**Wave Functions and Energies**					
	1		**2**		**3**	
	0.000 cm^{-1}		0.038 cm^{-1}		140.929 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	-0.177167+0.683929i	0.499	-0.177195+0.684058i	0.499	-0.004515-0.005123i	0.000
-5	-0.000543+0.000090i	0.000	-0.000463+0.000160i	0.000	0.405900-0.497248i	0.412
-4	0.004359-0.006520i	0.000	0.004733-0.006595i	0.000	-0.141764-0.101492i	0.030
-3	-0.011151+0.003903i	0.000	-0.011869+0.003724i	0.000	-0.096427+0.071537i	0.014
-2	0.007484+0.024037i	0.001	0.006306+0.018779i	0.000	0.078543+0.010467i	0.006
-1	0.003213-0.002651i	0.000	0.006171-0.003666i	0.000	0.032966-0.182179i	0.034
0	-0.000870-0.001124i	0.000	0.001617-0.001251i	0.000	-0.029541+0.065407i	0.005
1	0.003372-0.002446i	0.000	-0.005096+0.005055i	0.000	-0.114884+0.145181i	0.034
2	0.021392+0.013272i	0.001	-0.016598-0.010814i	0.000	-0.059781-0.052007i	0.006
3	-0.006575+0.009816i	0.000	0.006581-0.010556i	0.000	-0.010082-0.119641i	0.014
4	-0.007404+0.002585i	0.000	0.007571-0.002928i	0.000	0.169872+0.039257i	0.030
5	-0.000223+0.000503i	0.000	0.000271-0.000408i	0.000	-0.104699+0.633284i	0.412
6	0.706503	0.499	-0.706635	0.499	0.006829	0.000
M_J	**4**		**5**		**6**	
	141.845 cm^{-1}		183.925 cm^{-1}		193.038 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.006363+0.004153i	0.000	0.007223-0.015385i	0.000	-0.017494+0.007672i	0.000
-5	-0.339875+0.549805i	0.418	-0.206520-0.058031i	0.046	0.202291+0.183964i	0.075
-4	0.158758+0.100106i	0.035	0.050973-0.391528i	0.156	-0.132271+0.259087i	0.085
-3	0.010303-0.075420i	0.006	-0.335707-0.062081i	0.117	0.378590+0.139909i	0.163
-2	-0.099842-0.029896i	0.011	-0.004352+0.238762i	0.057	0.226995-0.116489i	0.065
-1	0.028552+0.134949i	0.019	-0.100717+0.123133i	0.025	-0.318359-0.086068i	0.109
0	0.143671+0.042735i	0.022	-0.238489-0.375440i	0.198	-0.081737+0.017135i	0.007
1	-0.097666+0.097405i	0.019	-0.154264+0.038837i	0.025	0.256990-0.206680i	0.109
2	-0.099950-0.029533i	0.011	0.217976+0.097534i	0.057	0.254667+0.015516i	0.065
3	0.032593-0.068790i	0.006	-0.086478+0.330264i	0.117	-0.290526+0.280178i	0.163
4	0.187661+0.002937i	0.035	-0.376072-0.120257i	0.156	-0.225189-0.184152i	0.085
5	-0.015871+0.646180i	0.418	-0.035240+0.211604i	0.046	-0.111377+0.249719i	0.075
6	0.007598	0.000	-0.016996	0.000	-0.019102	0.000
M_J	**7**		**8**		**9**	
	203.619 cm^{-1}		215.800 cm^{-1}		238.274 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.017164-0.008924i	0.000	-0.003281+0.004907i	0.000	-0.000996-0.009170i	0.000
-5	0.049326-0.036615i	0.004	0.134856+0.130711i	0.035	-0.000576-0.028060i	0.001
-4	-0.156546+0.198027i	0.064	-0.108379+0.032620i	0.013	0.585026-0.013817i	0.342
-3	-0.112524-0.102462i	0.023	-0.308109+0.018240i	0.095	-0.006061+0.076730i	0.006
-2	-0.152980+0.519227i	0.293	-0.048032-0.182322i	0.036	0.176071+0.086471i	0.038
-1	0.000986+0.171320i	0.029	-0.530616+0.032993i	0.283	-0.259480-0.210943i	0.112
0	0.098831+0.404317i	0.173	0.130646+0.244520i	0.077	-0.022371-0.020072i	0.001
1	-0.078158-0.152456i	0.029	-0.322369+0.422753i	0.283	0.237732+0.235181i	0.112
2	0.375257+0.390105i	0.293	-0.124863-0.141271i	0.036	0.104981+0.165702i	0.038
3	-0.052568+0.142817i	0.023	-0.186425+0.245988i	0.095	-0.075627+0.014312i	0.006
4	0.230247+0.103479i	0.064	0.087359-0.071962i	0.013	0.049445+0.583097i	0.342
5	0.060655+0.009731i	0.004	-0.033699-0.184759i	0.035	0.027958-0.002458i	0.001
6	-0.019345	0.000	0.005903	0.000	-0.009224	0.000

M_J	**10**		**11**		**12**	
	269.988 cm^{-1}		282.213 cm^{-1}		297.665 cm^{-1}	
	c	|c|	c	|c|	c	|c|
-6	0.004092-0.001654i	0.000	0.005200-0.005792i	0.000	-0.001437+0.011189i	0.000
-5	-0.064278-0.027067i	0.005	0.040244+0.012536i	0.002	-0.001440-0.014889i	0.000
-4	0.246939-0.338770i	0.176	-0.035463+0.153807i	0.025	-0.254257+0.025519i	0.065
-3	-0.041982+0.007671i	0.002	-0.369539-0.295262i	0.224	-0.078330-0.381089i	0.151
-2	-0.161557-0.073742i	0.032	0.146523+0.240716i	0.079	0.018506-0.386983i	0.150
-1	0.191142-0.150540i	0.059	-0.350181+0.197171i	0.162	0.282118+0.193783i	0.117
0	0.128535+0.661142i	0.454	-0.119720+0.053407i	0.017	0.133236-0.117220i	0.031
1	0.233622+0.067960i	0.059	0.380656-0.128857i	0.162	0.156268+0.304504i	0.117
2	0.122161-0.128900i	0.032	-0.081236-0.269841i	0.079	0.386188+0.030939i	0.150
3	-0.041798+0.008617i	0.002	0.027160-0.472230i	0.224	-0.368007-0.126235i	0.151
4	-0.355877-0.221575i	0.176	-0.138142-0.076362i	0.025	-0.057698+0.248935i	0.065
5	-0.049455+0.049178i	0.005	-0.017557+0.038321i	0.002	-0.014585-0.003324i	0.000
6	-0.004413	0.000	0.007784	0.000	-0.011281	0.000

M_J	**13**	
	301.375 cm^{-1}	
	c	|c|
-6	0.004032-0.006676i	0.000
-5	-0.030628-0.042077i	0.003
-4	-0.016500-0.092355i	0.009
-3	0.383504-0.227351i	0.199
-2	0.122673+0.465388i	0.232
-1	0.175023+0.142363i	0.051
0	-0.103999+0.058683i	0.014
1	0.031375+0.223418i	0.051
2	-0.334947-0.345609i	0.232
3	-0.392879+0.210737i	0.199
4	0.070525+0.061871i	0.009
5	-0.020183-0.047970i	0.003
6	0.007799	0.000

Table S14. Dipole transition strengths for $[Tb(TPP)(12C4)]^+$ obtained from RASSCF/RASSI/single_aniso calculations.

Basis Set 1						
From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	214	3.68×10^{-3}	1.36×10^{6}	2.94×10^{5}	1.33×10^{-9}	1.65×10^{6}
1	215	3.68×10^{-3}	2.94×10^{5}	1.36×10^{6}	5.01×10^{-9}	1.65×10^{6}
1	216	3.53×10^{-3}	2.55×10^{5}	1.33×10^{6}	7.20×10^{-9}	1.59×10^{6}
1	217	3.53×10^{-3}	1.33×10^{6}	2.55×10^{5}	5.61×10^{-9}	1.59×10^{6}
1	508	2.92	2.40×10^{9}	2.13×10^{-9}	1.83×10^{-7}	4.53×10^{9}
1	509	2.92	2.13×10^{9}	2.40×10^{-9}	7.96×10^{-9}	4.53×10^{9}
1	510	2.79	9.45E+07	4.24×10^{-9}	7.60×10^{-8}	4.34×10^{9}
1	511	2.79	4.24×10^{9}	9.46×10^{7}	3.86×10-^{9}	4.34×10^{9}

Basis Set 2						
From	To	Oscillator Strength	Einstein Coefficient (sec^{-1})			Total A (sec^{-1})
			A_x	A_y	A_z	
1	212	3.83×10^{-3}	4.63×10^{5}	1.27×10^{6}	2.08×10^{-10}	1.74×10^{6}
1	213	3.82×10^{-3}	1.27×10^{6}	4.63×10^{5}	1.10×10^{-8}	1.74×10^{6}
1	214	3.70×10^{-3}	1.13×10^{6}	5.54×10^{5}	1.31×10^{-8}	1.68×10^{6}

1	215	3.70×10^{-3}	5.53×10^{5}	1.13×10^{6}	1.79×10^{-9}	1.68×10^{6}
1	510	2.88	2.17×10^{9}	2.32×10^{9}	2.66×10^{-8}	4.49×10^{9}
1	511	2.87	2.32×10^{9}	2.17×10^{9}	6.10×10^{-9}	4.49×10^{9}
1	514	2.71	2.78×10^{9}	1.45×10^{9}	3.81×10^{-7}	4.23×10^{9}
1	515	2.71	1.45×10^{9}	2.78×10^{9}	1.24×10^{-9}	4.23×10^{9}

Table S15. Low-Lying Spin Orbit of $[Tb(TPP)(12C4)]^{+}$ obtained from RASSCF/RASSI/single_aniso calculations.

Basis Set 1						
S.O states	Energy (cm^{-1})	g_z	g_x	g_y	L_z	S_z
1	0.00	17.98	0.00	0.00	2.99	2.99
2	0.11					
214	25962.06	26.21	0.00	0.00	7.11	2.99
215	25962.07					
216	25971.45	9.65	0.00	0.00	-1.16	2.99
217	25971.45					
508	48259.89	18.18	0.00	0.00	3.10	2.99
509	48259.89					
510	48269.40	17.72	0.00	0.00	2.87	2.99
511	48269.40					
Basis Set 2						
S.O states	Energy (cm^{-1})	g_z	g_x	g_y	L_z	S_z
1	0.00	17.98	0.00	0.00	2.99	2.99
2	0.08					
212	26093.63	26.13	0.00	0.00	7.10	2.99
213	26093.63					
214	26101.24	9.69	0.00	0.00	-1.14	2.99
215	26101.24					
510	48396.49	18.16	0.00	0.00	3.12	2.98
511	48396.49					
514	48404.49	17.47	0.00	0.00	2.82	2.96
515	48404.49					