Supporting Information

Electronic Structure and Photophysics of (C=C)tetra-*p*-tolylporphyrin^{2+}

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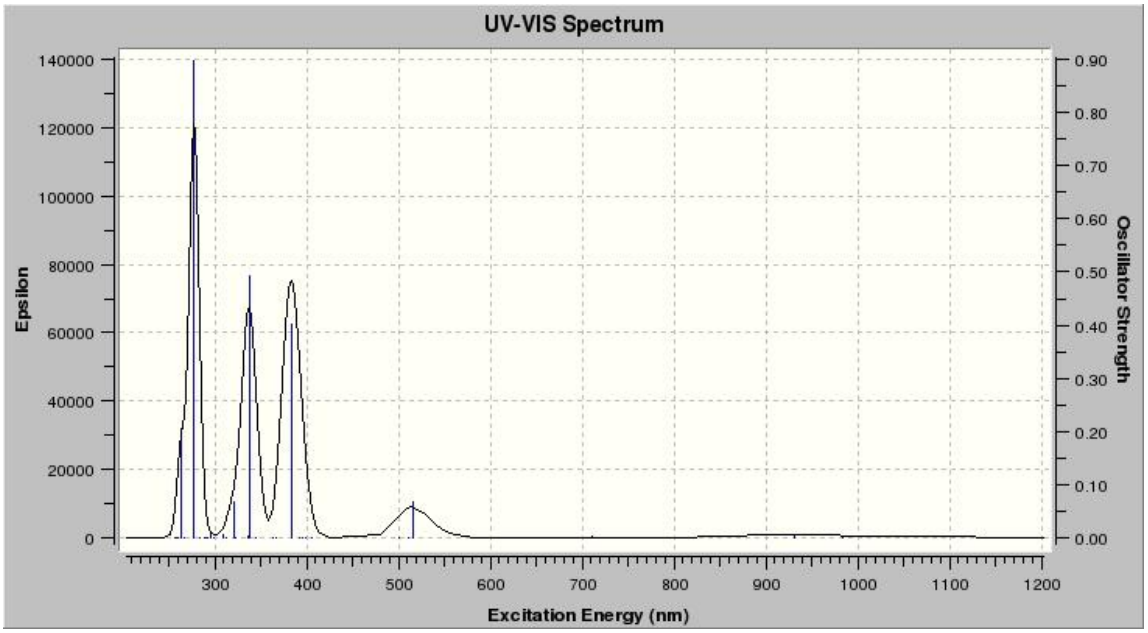
Figure S1. Calculated Gas Phase (TD-DFT, B3LYP/DZVP2) Absorption Spectra.

A. Ruffled (C=C)porphine^{2+}



B. (C=C)TTP^{2+}

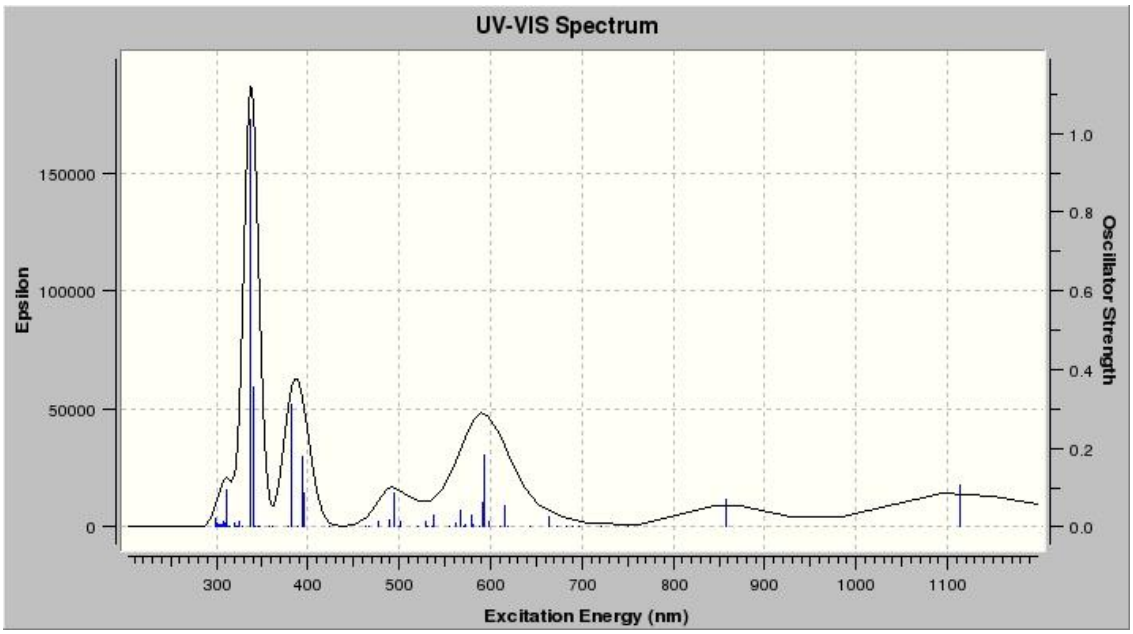
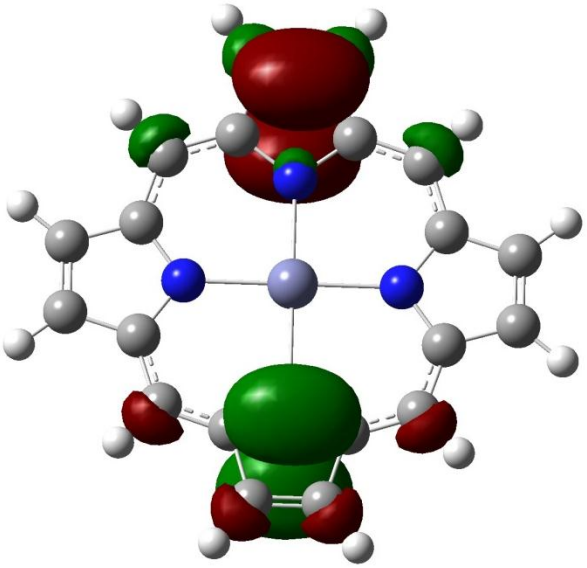
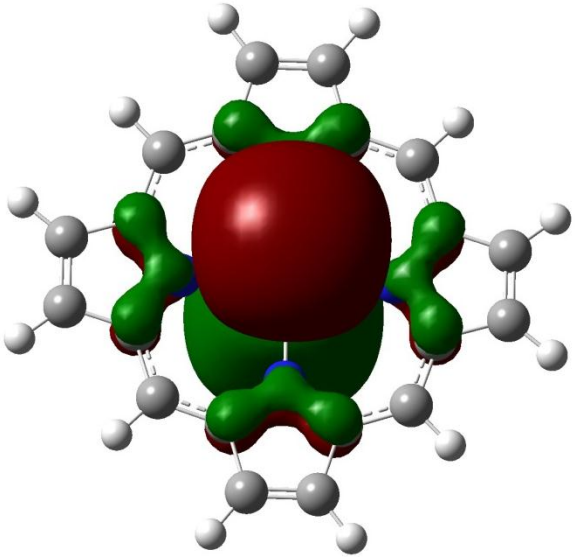
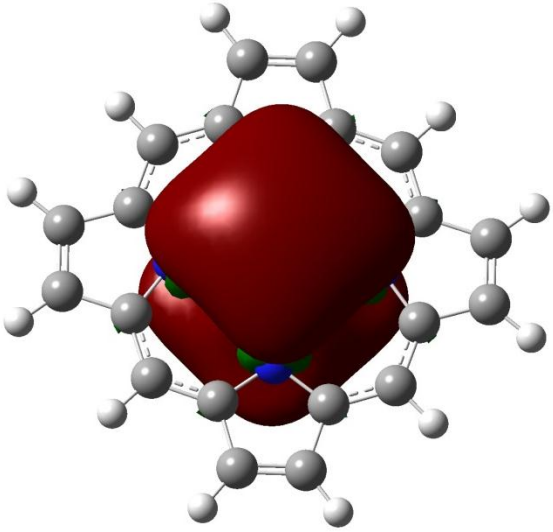
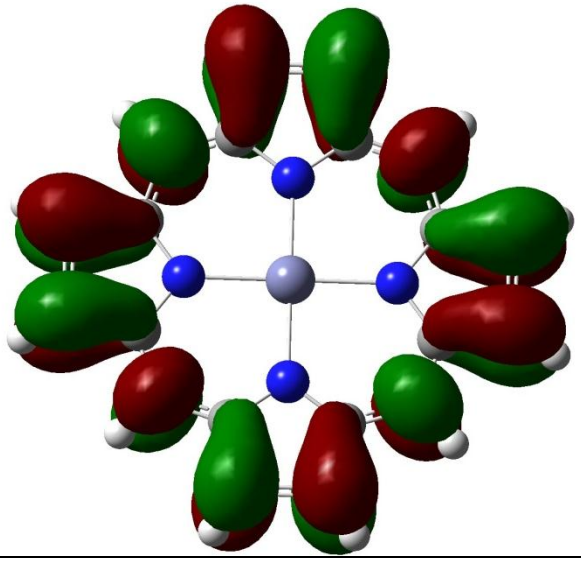
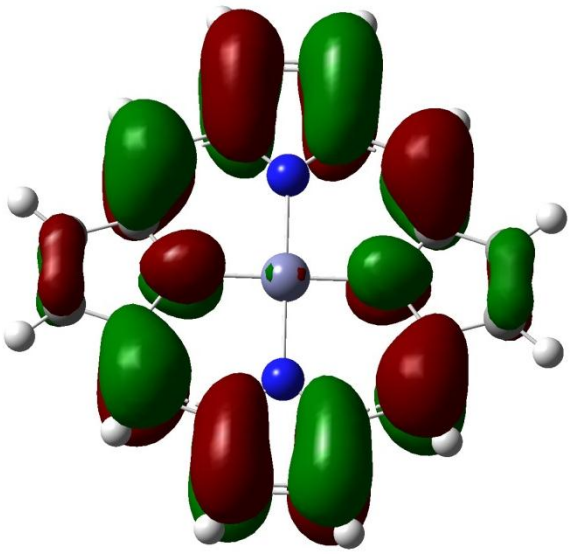
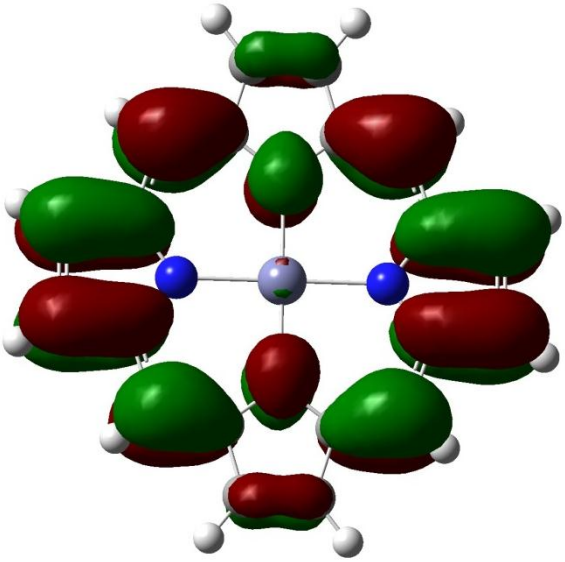
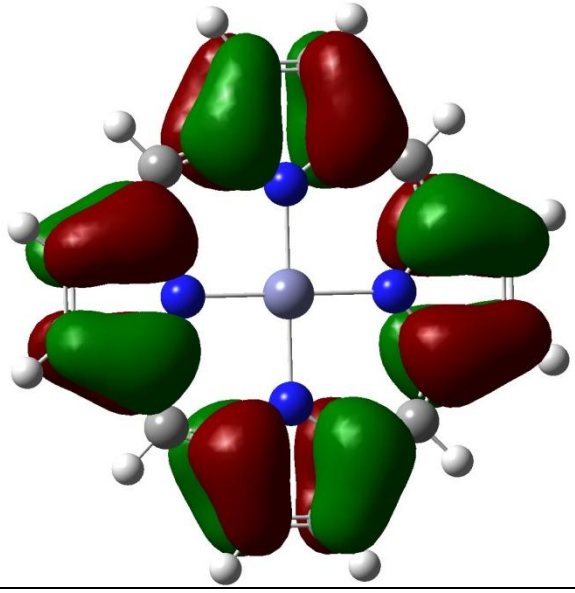
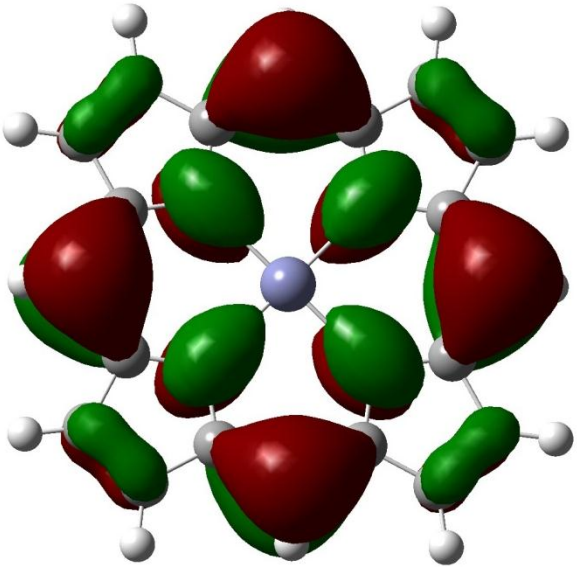
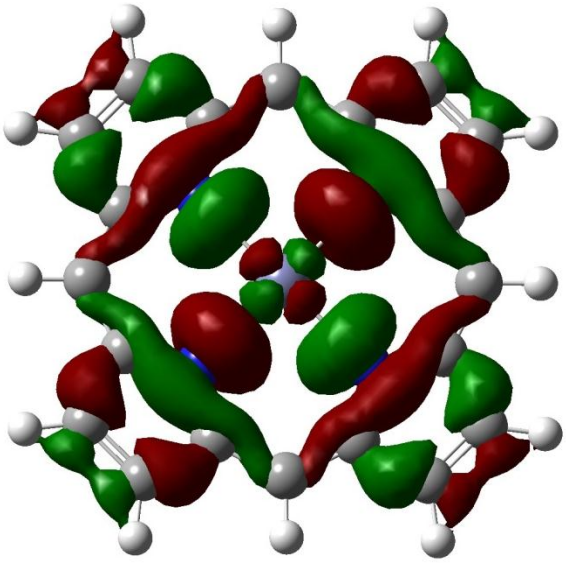
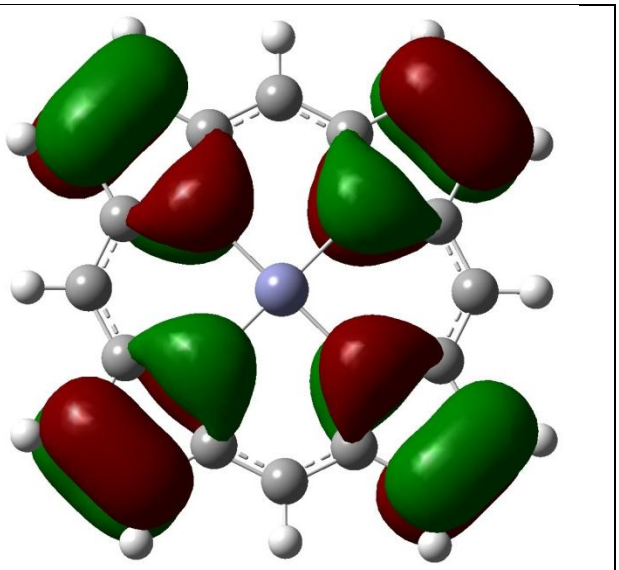
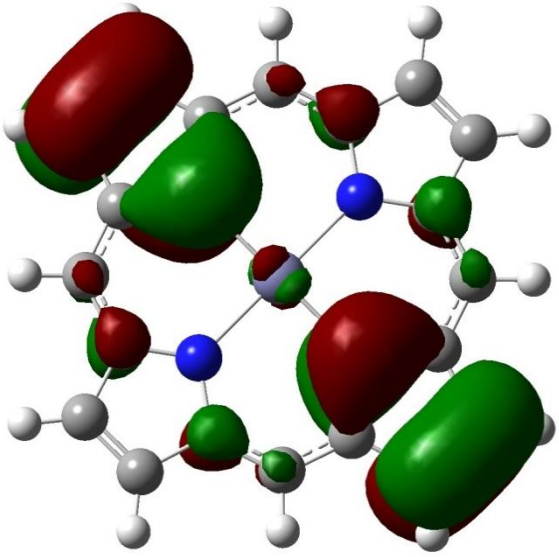
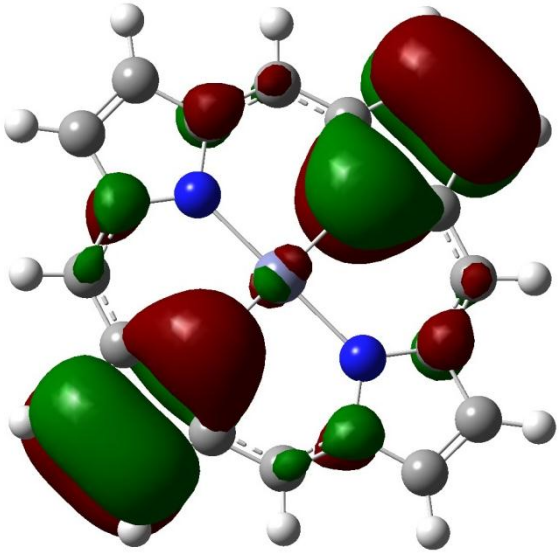


Table S1. Orbitals Pictures and Energies (LUMO+5 – HOMO-5).

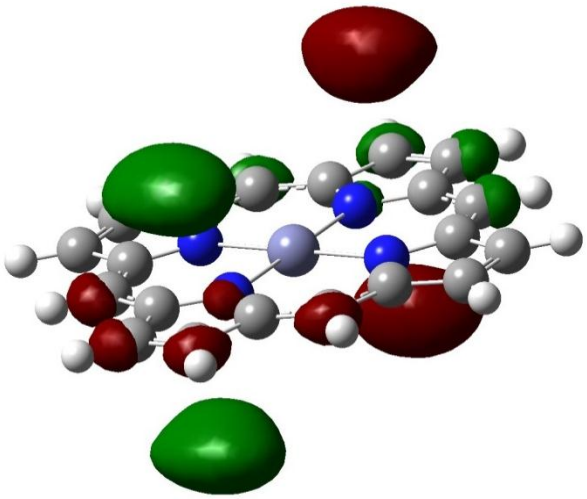
A. Zn(porphine)

	
LUMO+5 (0.41 eV)	LUMO+4 (0.21 eV)
	
LUMO+3 (0.05 eV)	LUMO+2 (-0.92 eV)

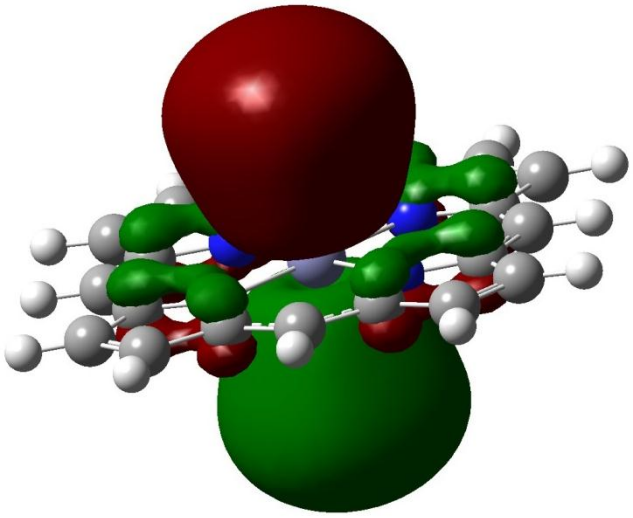
	
LUMO+1 (-2.51 eV)	LUMO (-2.51 eV)
	
HOMO (-5.54 eV)	HOMO-1 (-5.54 eV)

	
HOMO-2 (-6.80 eV)	HOMO-3 (-6.89 eV)
	
HOMO-4 (-6.92 eV)	HOMO-5 (-6.92 eV)

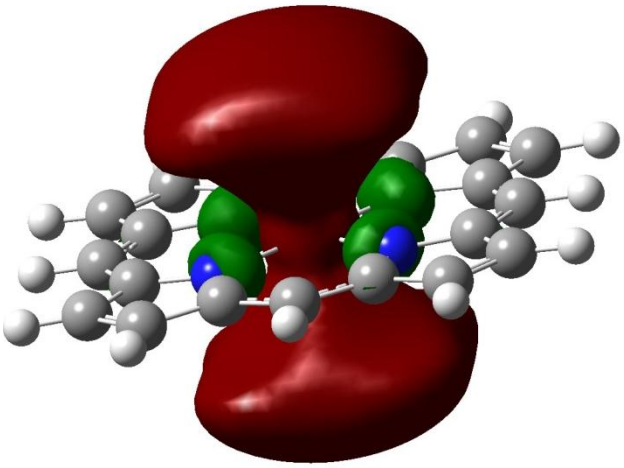
A.1. Zn(porphine) different images for LUMO+5 – LUMO+3



LUMO+5 (0.41 eV)

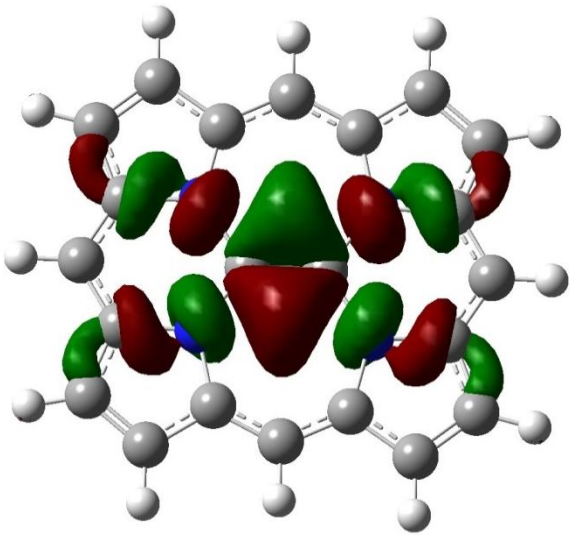
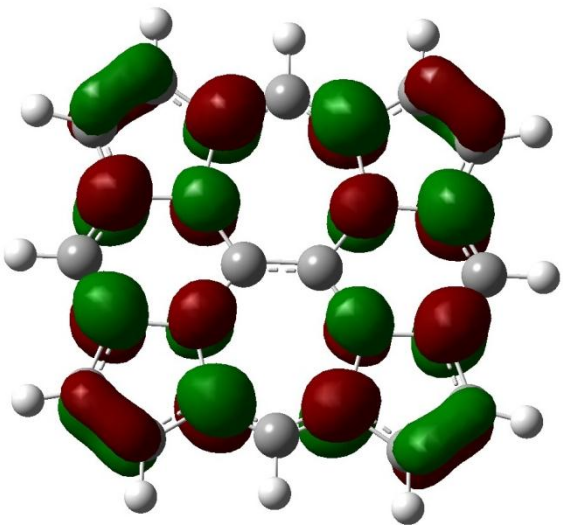
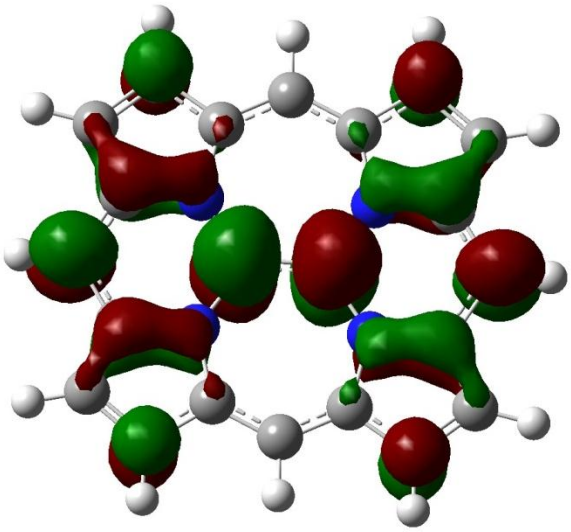
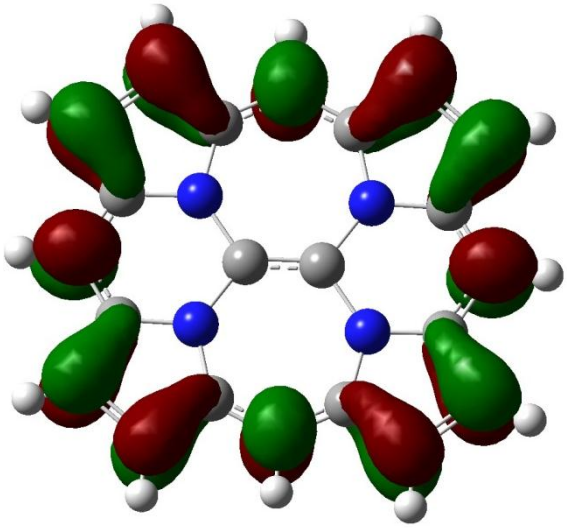


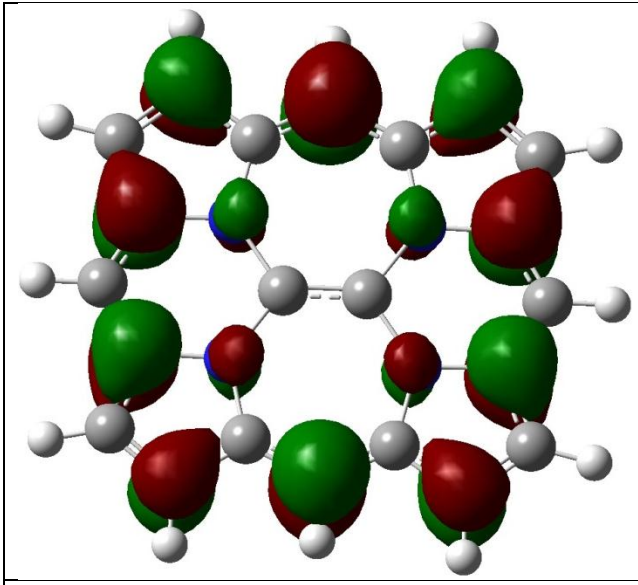
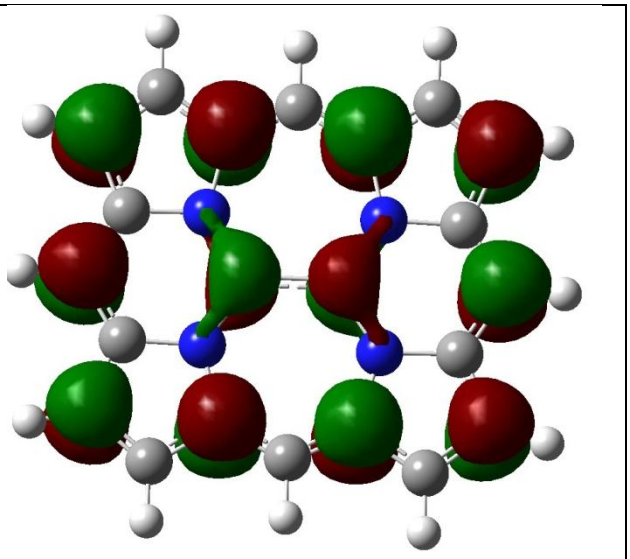
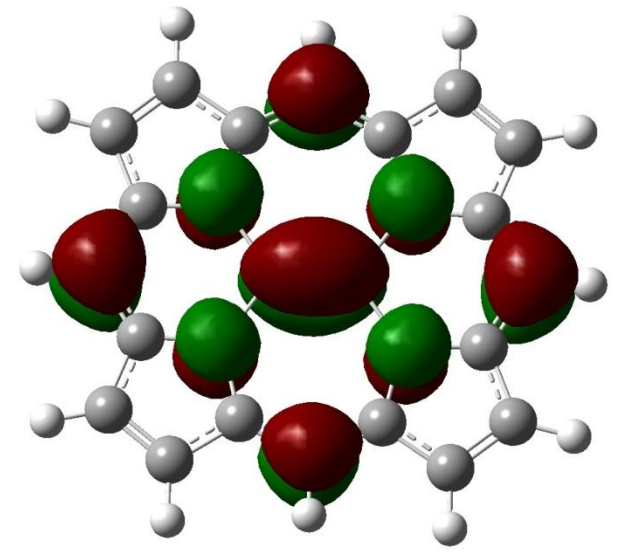
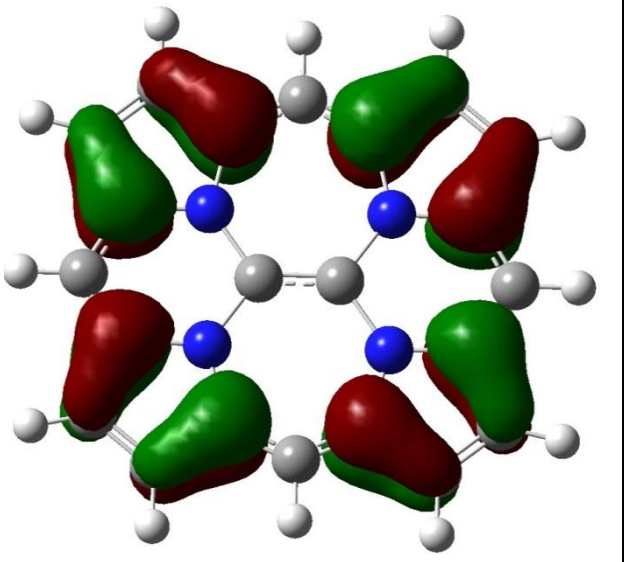
LUMO+4 (0.21 eV)

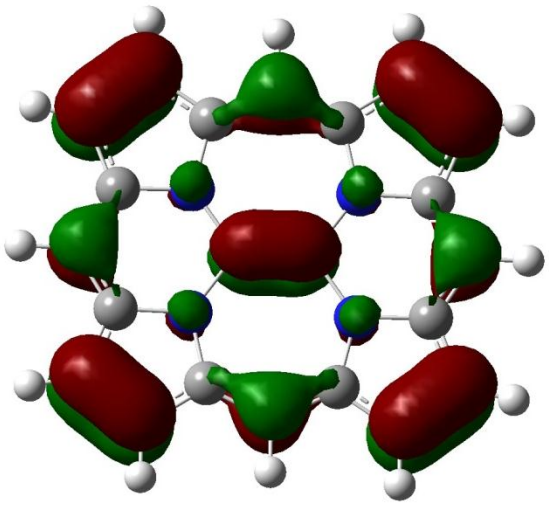
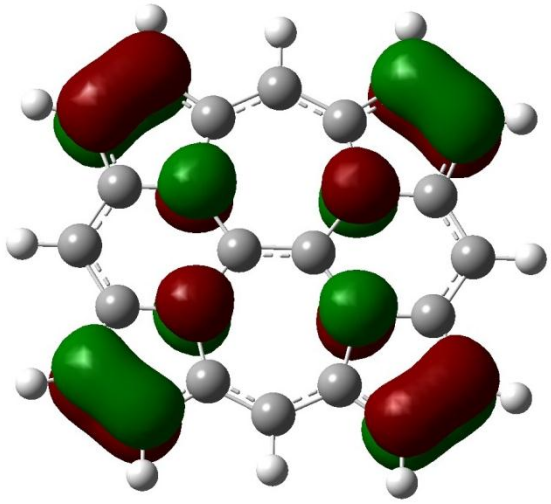
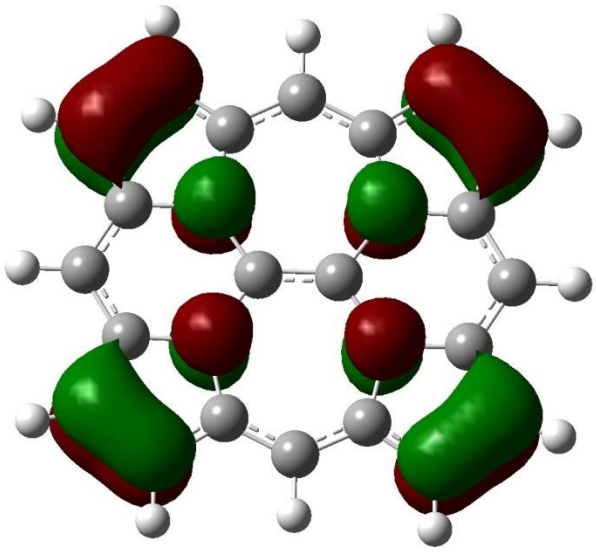
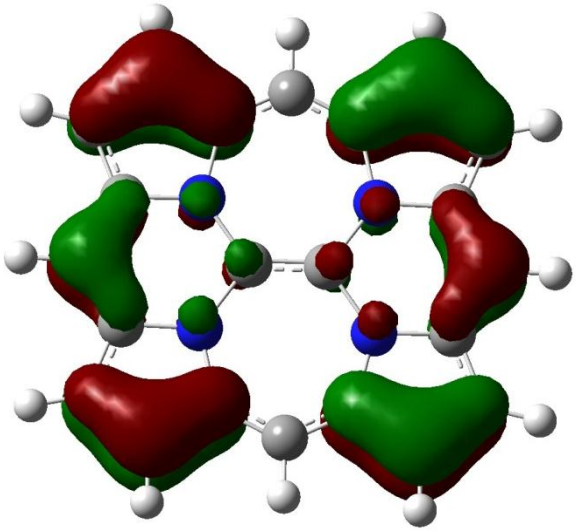


LUMO+3 (0.05 eV)

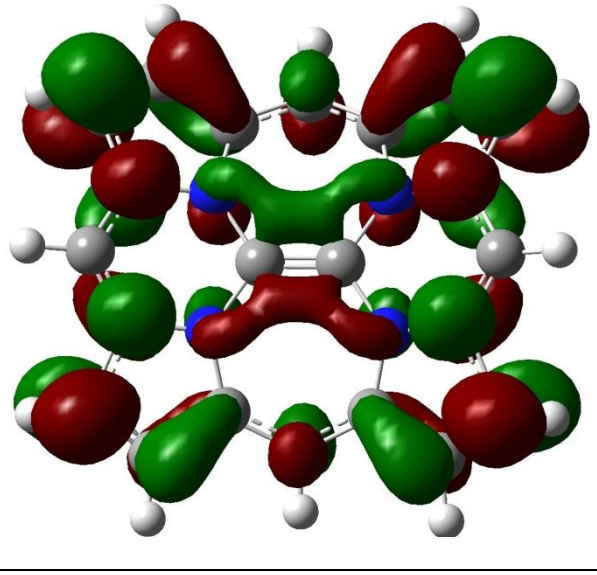
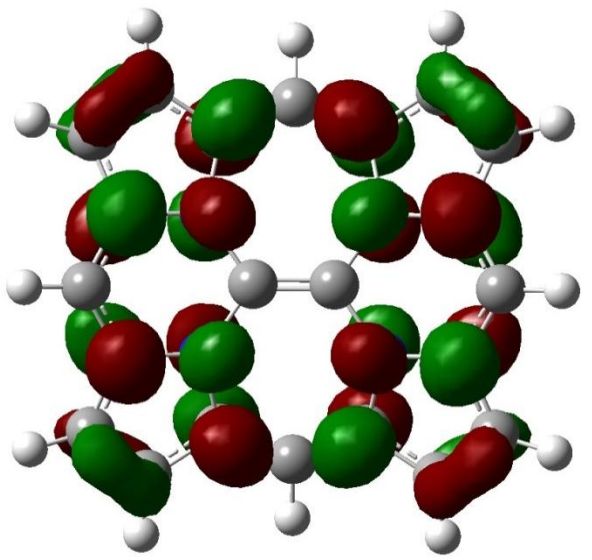
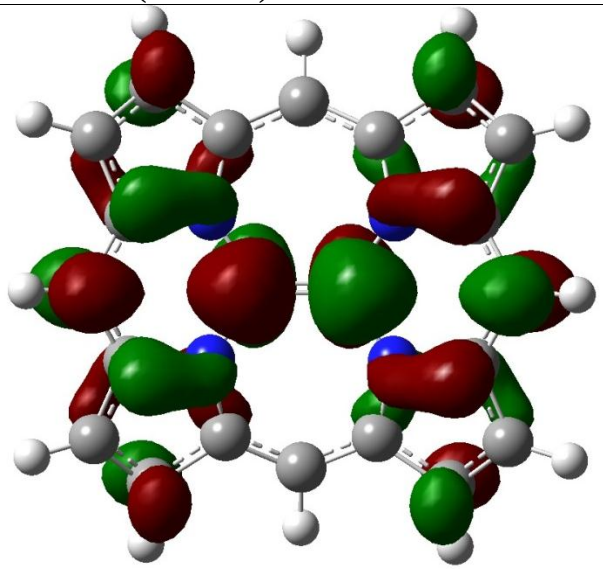
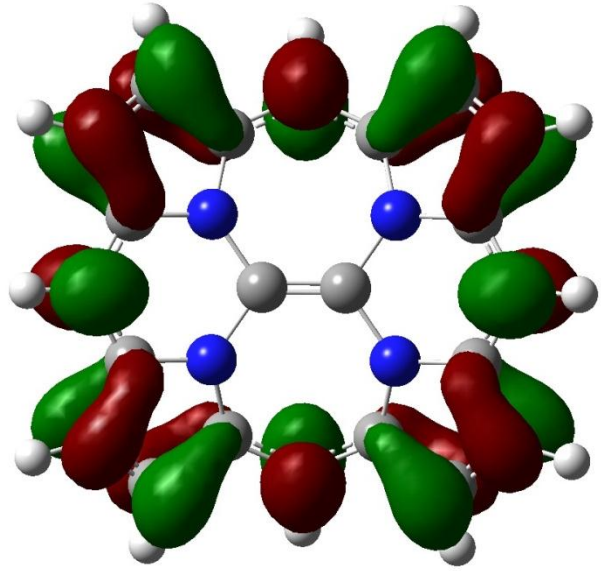
B. Planar (C=C)porphine^{2+} (8.5 kcal/mol higher in energy than the ruffled (C=C)porphine^{2+})

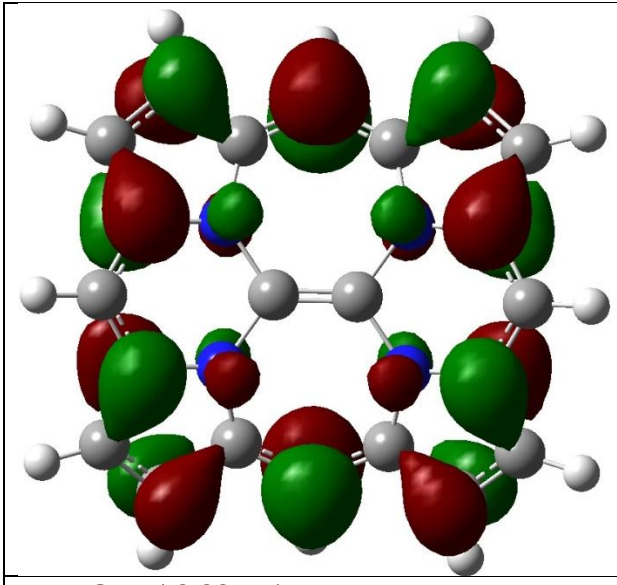
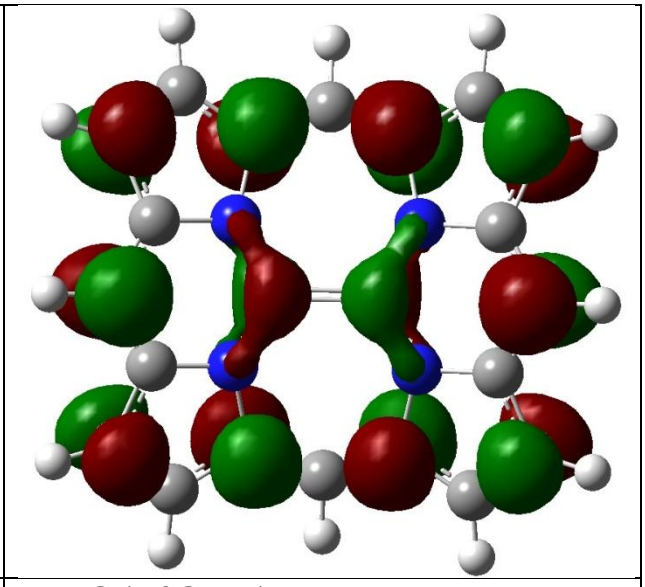
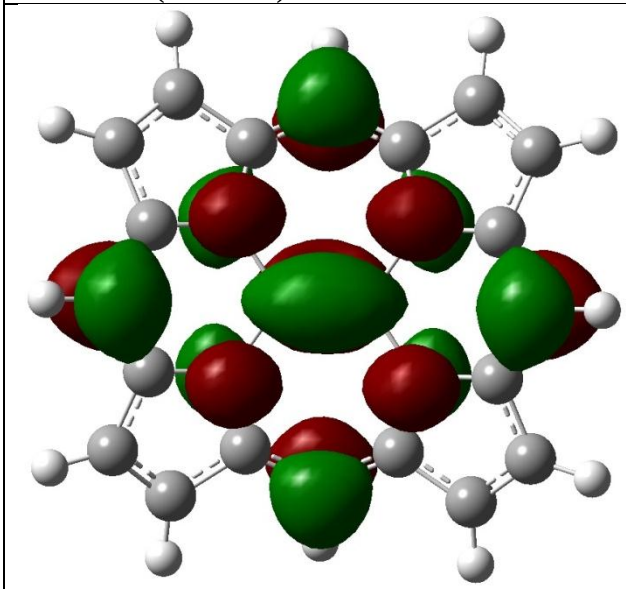
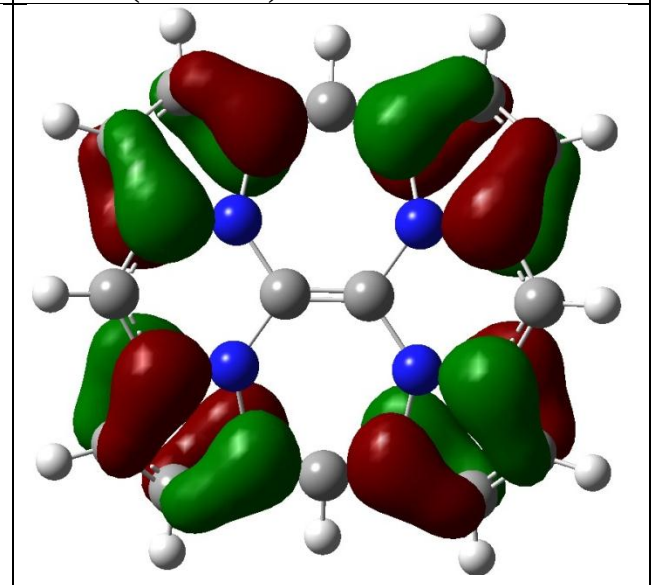
	
LUMO+5 (-5.96 eV)	LUMO+4 (-6.99 eV)
	
LUMO+3 (-7.55 eV)	LUMO+2 (-7.88 eV)

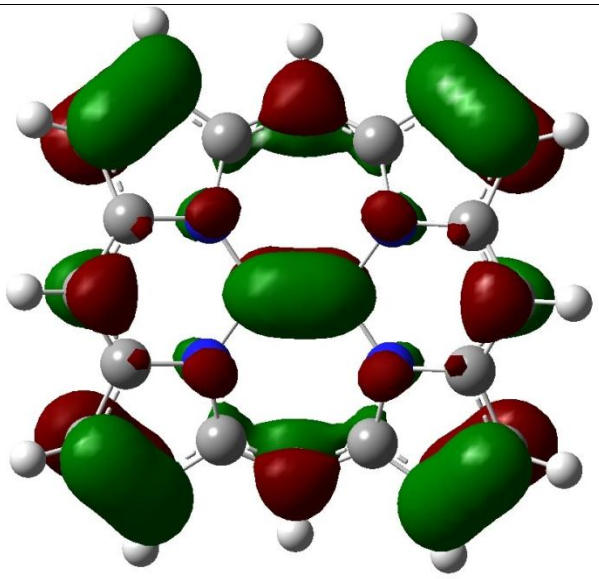
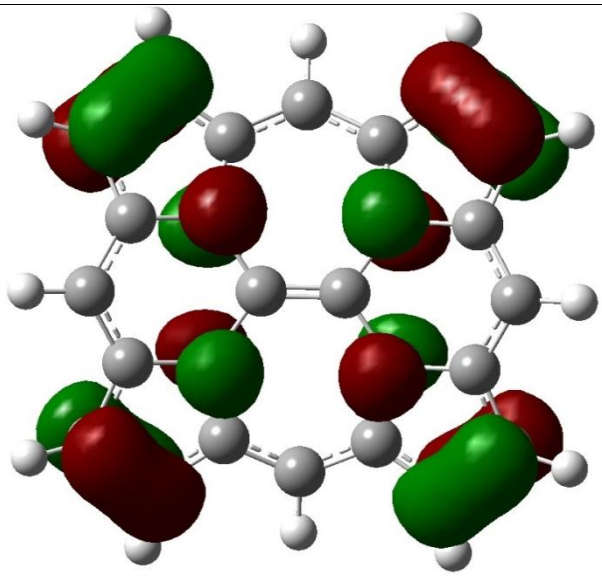
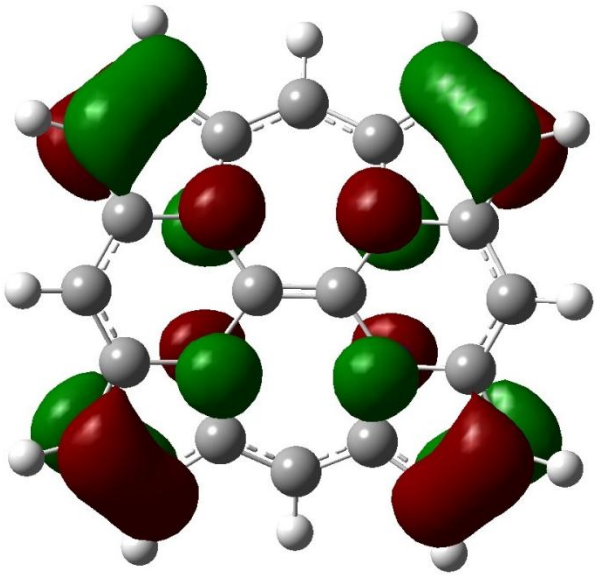
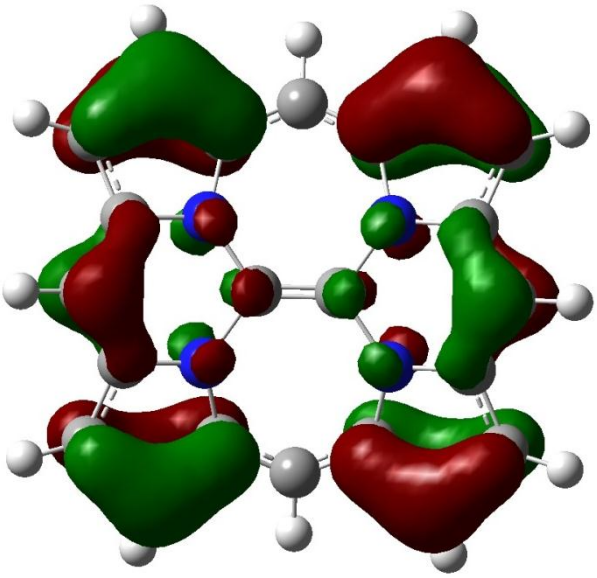
	
LUMO+1 (-9.90 eV)	LUMO (-10.37 eV)
	
HOMO (-12.23 eV)	HOMO-1 (-13.00 eV)

	
HOMO-2 (-13.52 eV)	HOMO-3 (-14.53 eV)
	
HOMO-4 (-14.62 eV)	HOMO-5 (-15.07 eV)

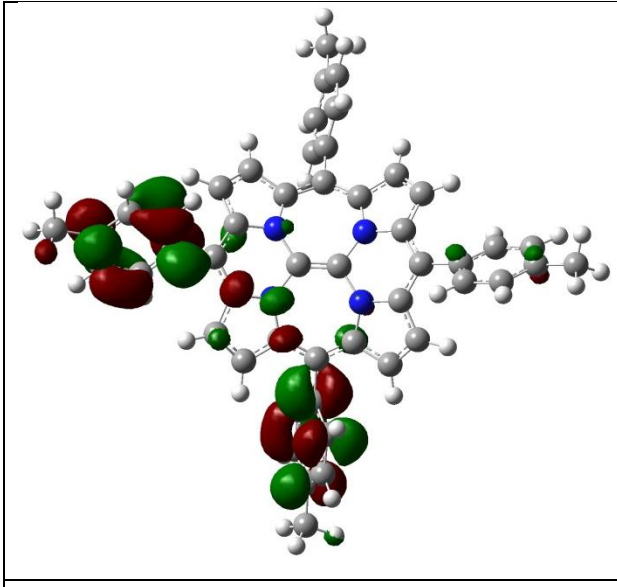
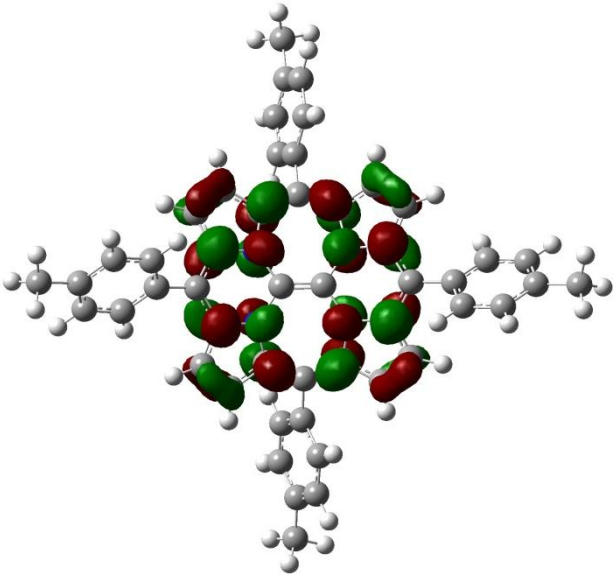
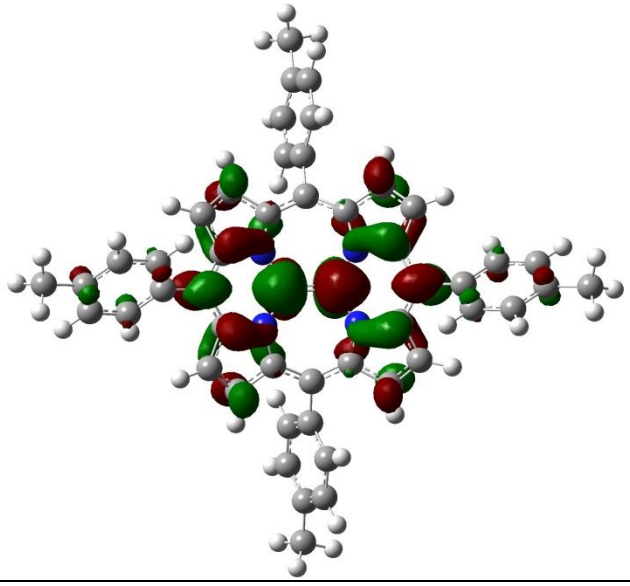
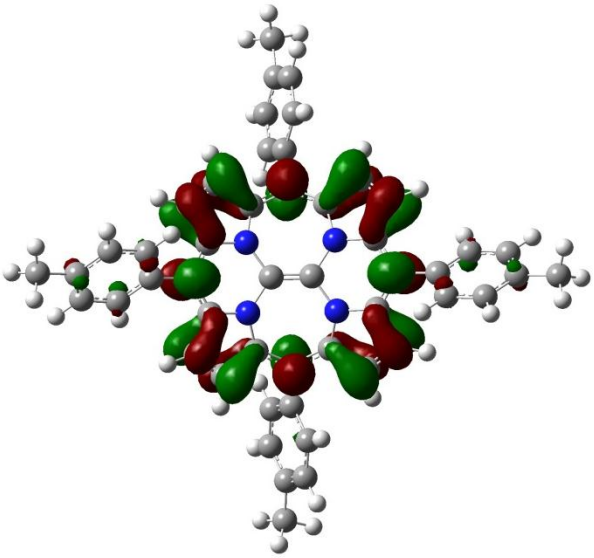
C. Ruffled (C=C)porphine^{2+}

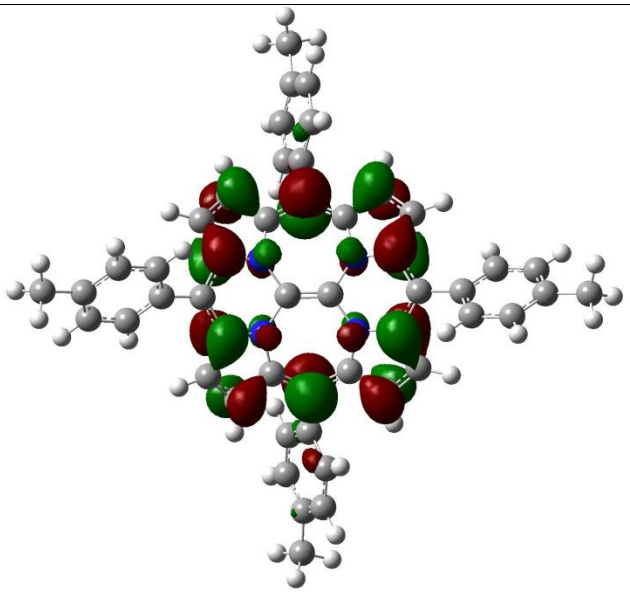
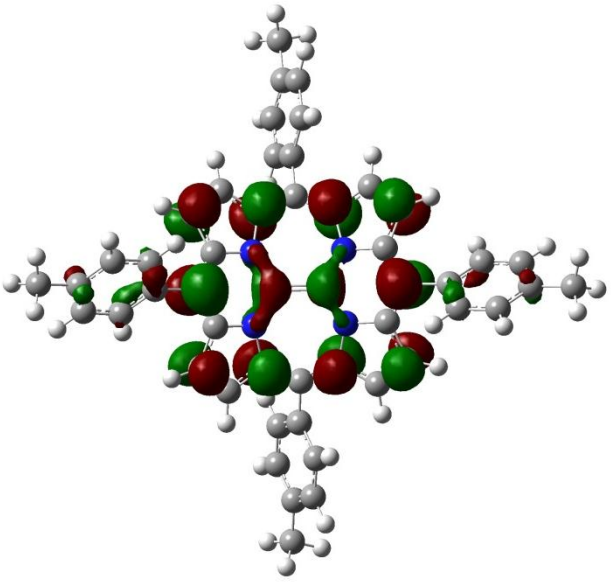
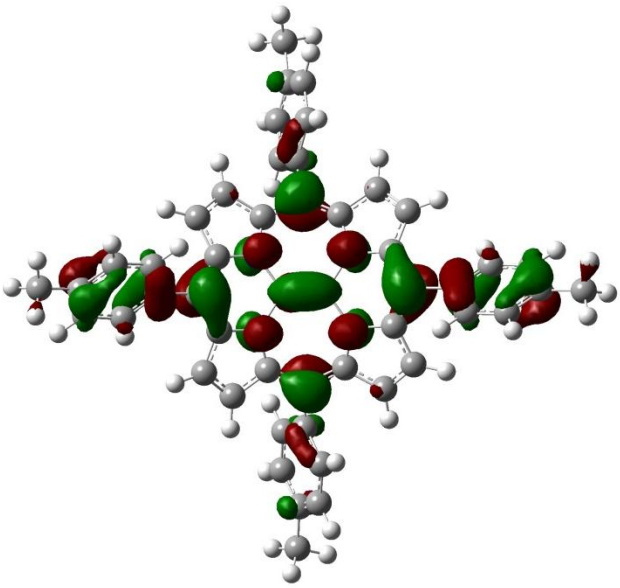
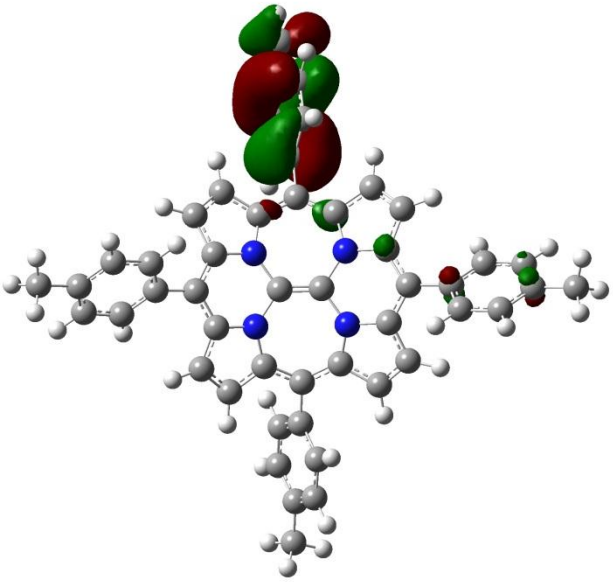
	
LUMO+5 (-5.89 eV)	LUMO+4 (-6.95 eV)
	
LUMO+3 (-7.65 eV)	LUMO+2 (-8.09 eV)

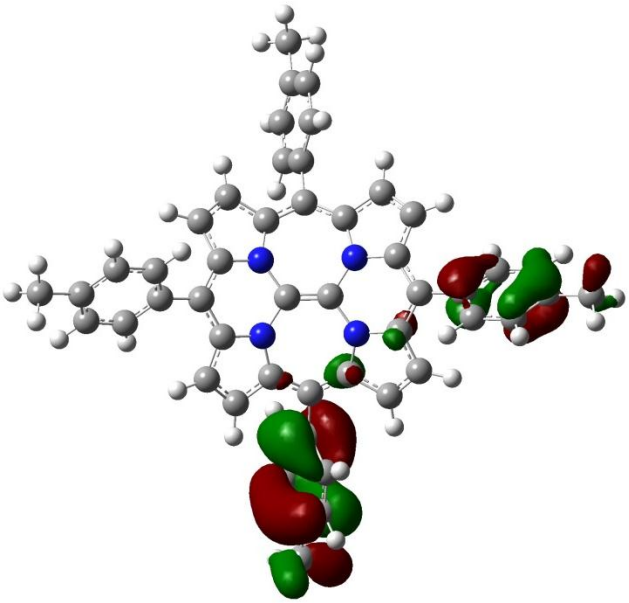
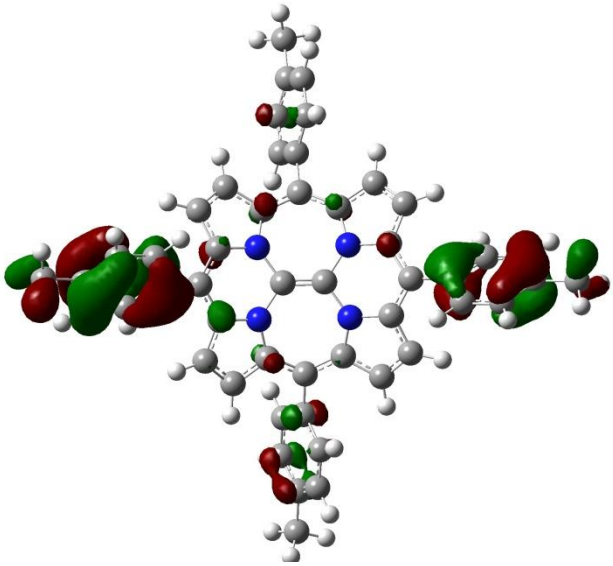
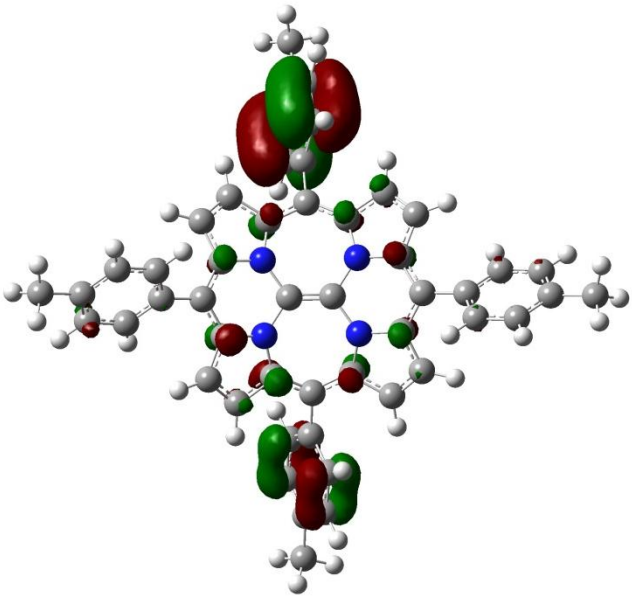
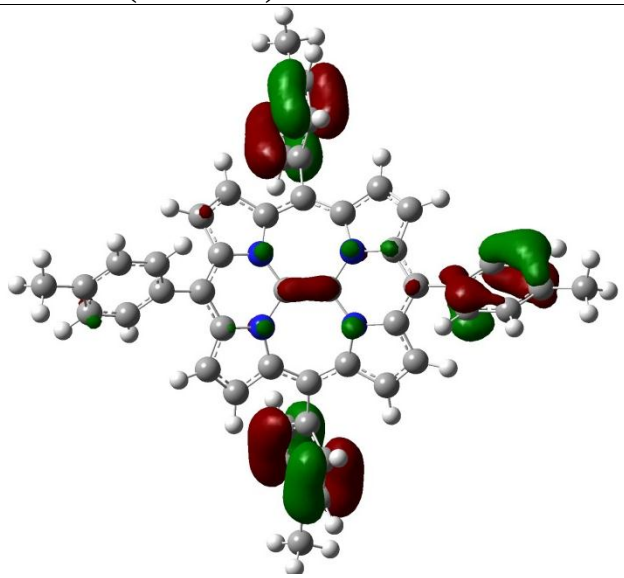
	
LUMO+1 (-9.98 eV)	LUMO (-10.35 eV)
	
HOMO (-12.39 eV)	HOMO-1 (-13.03 eV)

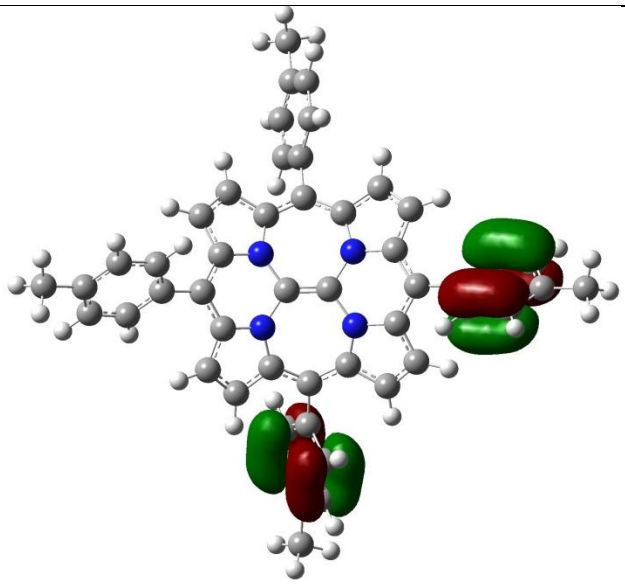
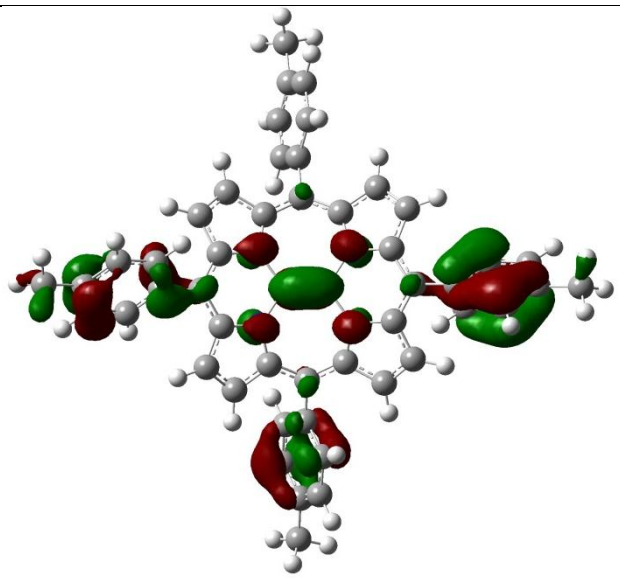
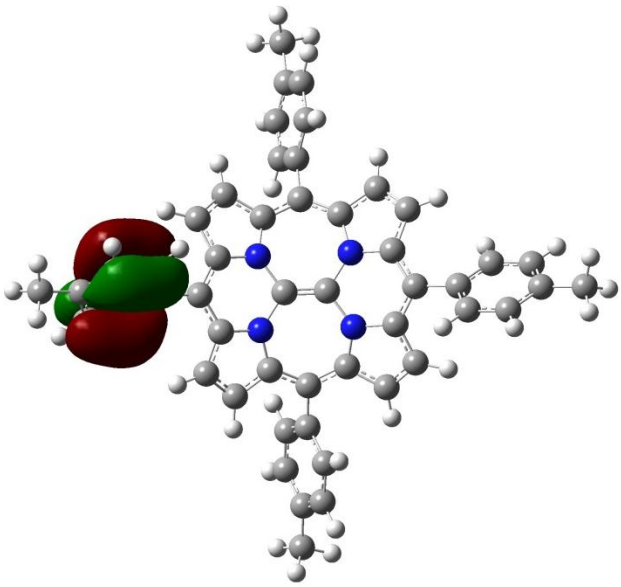
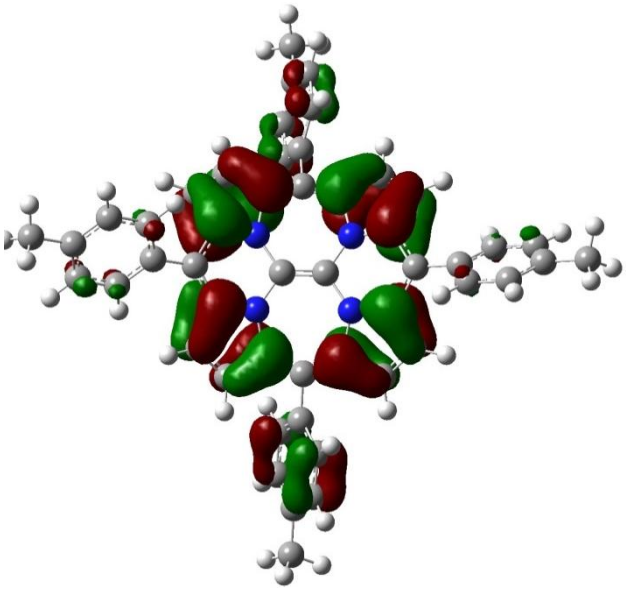
	
HOMO-2 (-13.52 eV)	HOMO-3 (-14.43 eV)
	
HOMO-4 (-14.56 eV)	HOMO-5 (-15.03 eV)

D. (C=C)TTP^{2+}

	
LUMO+5 (-5.16 eV)	LUMO+4 (-5.63 eV)
	
LUMO+3 (-6.40 eV)	LUMO+2 (-6.91 eV)

	
LUMO+1 (-8.62 eV)	LUMO (-8.92 eV)
	
HOMO (-10.51 eV)	HOMO-1 (-11.19 eV)

	
HOMO-2 (-11.23 eV)	HOMO-3 (-11.28 eV)
	
HOMO-4 (-11.43 eV)	HOMO-5 (-11.51 eV)

	
HOMO-6 (-11.54 eV)	HOMO-7 (-11.56 eV)
	
HOMO-8 (-11.59 eV)	HOMO-9 (-11.80 eV)

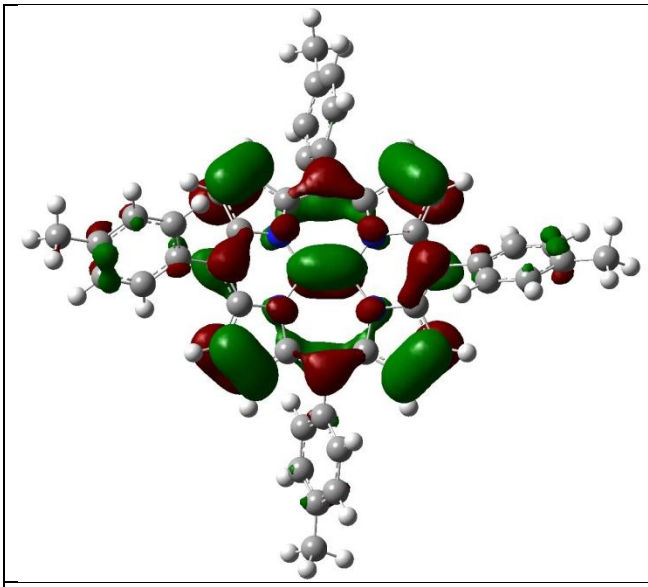
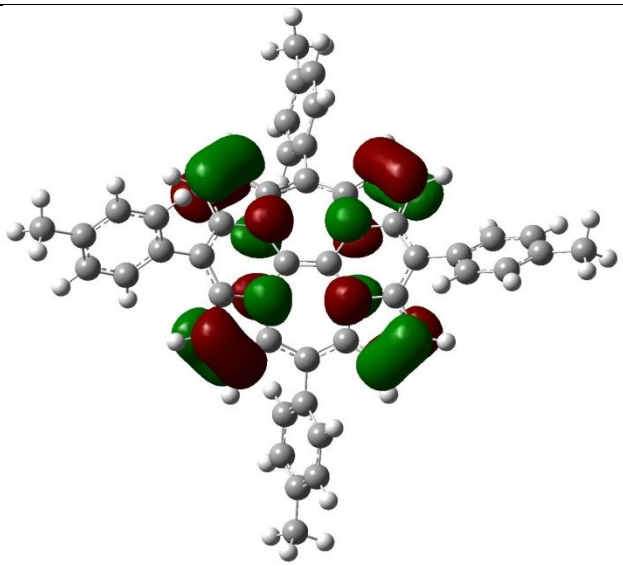
	
HOMO-10 (-12.19 eV)	HOMO-11 (-13.07 eV)

Table S2. Excitation Energies Determined using Gaussian '09: Gas Phase vs CH_2Cl_2 solution.

A. Planar (C=C)porphine^{2+}:

Gas						CH_2Cl_2				
	symm	**eV**	**nm**	**f**			**symm**	**eV**	**nm**	**f**
1	$^1B_{1U}$	1.1374	1090.1	0.006		1	$^1B_{1U}$	1.0491	1181.8	0.009
2	$^1B_{2U}$	1.6737	740.8	0.004		2	$^1B_{2U}$	1.5950	777.3	0.011
3	$^1B_{2U}$	2.3628	524.8	0.078		3	$^1B_{2U}$	2.3067	537.5	0.160
4	$^1B_{1U}$	2.4514	505.8	0.001		4	$^1B_{1U}$	2.4588	504.2	0.000
5	$^1B_{1U}$	3.2786	378.2	0.404		5	$^1B_{1U}$	3.1669	391.5	0.757
6	$^1B_{2U}$	3.3156	374.0	0.159		6	$^1B_{2U}$	3.2858	377.3	0.343
7	$^1B_{3G}$	3.6498	339.7	0.000		7	^1A_G	3.6310	341.5	0.000
8	^1A_G	3.7449	331.1	0.000		8	$^1B_{3G}$	3.6418	340.5	0.000
9	$^1B_{2U}$	3.7763	328.3	0.497		9	$^1B_{2U}$	3.6853	336.4	0.590
10	$^1B_{1U}$	4.0642	305.1	0.074		10	$^1B_{1U}$	4.0527	305.9	0.206
11	^1A_G	4.1623	297.9	0.000		11	^1A_G	4.1633	297.8	0.000
12	^1A_G	4.2263	293.4	0.000		12	^1A_G	4.2227	293.6	0.000
13	$^1B_{3G}$	4.3217	286.9	0.000		13	$^1B_{3G}$	4.2915	288.9	0.000
14	$^1B_{3G}$	4.4388	279.3	0.000		14	$^1B_{1U}$	4.3039	288.1	1.182
15	$^1B_{1U}$	4.5326	273.5	1.123		15	$^1B_{3G}$	4.3744	283.4	0.000
16	$^1B_{3G}$	4.5690	271.4	0.000		16	$^1B_{3G}$	4.5451	272.8	0.000
17	^1A_G	4.8484	255.7	0.000		17	^1A_G	4.7937	258.6	0.000
18	$^1B_{2U}$	4.8528	255.5	0.341		18	$^1B_{2U}$	4.8372	256.3	0.374
19	$^1B_{3G}$	4.9552	250.2	0.000		19	$^1B_{3G}$	4.8763	254.3	0.000
20	^1A_G	5.0093	247.5	0.000		20	^1A_G	4.9770	249.1	0.000
21	$^1B_{1G}$	5.0753	244.3	0.000		21	$^1B_{1G}$	5.0814	244.0	0.000
22	^1A_G	5.2544	236.0	0.000		22	^1A_G	5.2217	237.4	0.000
23	$^1B_{3G}$	5.2869	234.5	0.000		23	$^1B_{3G}$	5.2245	237.3	0.000
24	$^1B_{1U}$	5.3730	230.8	0.049		24	$^1B_{1U}$	5.4134	229.0	0.028

25	$^1B_{1U}$	5.7062	217.3	0.014		25	$^1B_{2U}$	5.5858	222.0	0.004
26	$^1B_{2U}$	5.7203	216.8	0.005		26	$^1B_{1U}$	5.6698	218.7	0.018
27	^1A_G	5.8221	213.0	0.000		27	^1A_G	5.7254	216.6	0.000
28	$^1B_{1U}$	6.0236	205.8	0.000		28	$^1B_{1U}$	5.9478	208.5	0.003
29	$^1B_{3G}$	6.0884	203.6	0.000		29	$^1B_{3G}$	6.0585	204.6	0.000
30	$^1B_{3G}$	6.1407	201.9	0.000		30	$^1B_{3G}$	6.0860	203.7	0.000
31	^1A_U	6.1490	201.6	0.000		31	$^1B_{2U}$	6.1336	202.1	0.009
32	$^1B_{2G}$	6.1673	201.0	0.000		32	^1A_U	6.1374	202.0	0.000
33	$^1B_{2U}$	6.1723	200.9	0.006		33	$^1B_{2U}$	6.1766	200.7	0.081
34	$^1B_{1G}$	6.1861	200.4	0.000		34	$^1B_{1G}$	6.1806	200.6	0.000
35	$^1B_{2U}$	6.2101	199.7	0.069		35	$^1B_{3G}$	6.1982	200.0	0.000
36	$^1B_{1G}$	6.2177	199.4	0.000		36	$^1B_{1G}$	6.2144	199.5	0.000
37	$^1B_{3U}$	6.2801	197.4	0.000		37	$^1B_{2G}$	6.2559	198.2	0.000
38	$^1B_{3G}$	6.3563	195.1	0.000		38	$^1B_{3U}$	6.2753	197.6	0.000
39	$^1B_{2U}$	6.3722	194.6	0.308		39	$^1B_{1U}$	6.3621	194.9	0.843
40	$^1B_{3G}$	6.4689	191.7	0.000		40	$^1B_{2U}$	6.3760	194.5	0.311

B. Ruffled (C=C)porphine^{2+}

Gas						**CH_2Cl_2**				
	symm	eV	nm	f			symm	eV	nm	f
1	$^1B_2$	1.3315	931.1	0.007		1	$^1B_2$	1.2357	1003.3	0.013
2	$^1B_1$	1.7421	711.7	0.004		2	$^1B_1$	1.6606	746.6	0.010
3	$^1B_1$	2.4012	516.3	0.067		3	$^1B_1$	2.3454	528.6	0.147
4	$^1B_2$	2.4272	510.8	0.000		4	$^1B_2$	2.4314	509.9	0.001
5	$^1B_2$	3.2346	383.3	0.402		5	$^1B_2$	3.1213	397.2	0.738
6	$^1B_1$	3.2374	383.0	0.156		6	$^1B_1$	3.2013	387.3	0.345
7	$^1A_2$	3.5998	344.4	0.000		7	$^1A_1$	3.5656	347.7	0.007
8	$^1B_1$	3.6748	337.4	0.493		8	$^1B_1$	3.5806	346.3	0.544
9	$^1A_1$	3.6821	336.7	0.003		9	$^1A_2$	3.5941	345.0	0.000
10	$^1B_2$	3.8655	320.8	0.068		10	$^1B_2$	3.8630	321.0	0.113

11	$^1A_1$	4.0114	309.1	0.005		11	$^1A_1$	4.0155	308.8	0.007
12	$^1A_1$	4.1888	296.0	0.005		12	$^1A_1$	4.1860	296.2	0.007
13	$^1A_2$	4.2789	289.8	0.000		13	$^1A_2$	4.2446	292.1	0.000
14	$^1A_2$	4.3608	284.3	0.000		14	$^1B_2$	4.2715	290.3	1.021
15	$^1B_2$	4.4685	277.5	0.898		15	$^1A_2$	4.3433	285.5	0.000
16	$^1A_2$	4.6396	267.2	0.000		16	$^1A_2$	4.5753	271.0	0.000
17	$^1B_1$	4.7032	263.6	0.207		17	$^1A_1$	4.6982	263.9	0.001
18	$^1A_1$	4.7032	260.8	0.000		18	$^1B_1$	4.7004	262.7	0.223

C. (C=C)porphine^0

Gas						**CH_2Cl_2**				
	symm	eV	nm	f			symm	eV	nm	f
1	^1A	0.7707	1608.7	0.000		1	^1A	0.7901	1569.2	0.000
2	^1B	1.7423	711.6	0.012		2	^1B	1.7511	708.0	0.023
3	^1B	2.5738	481.7	0.085		3	^1B	2.5772	481.1	0.178
4	^1B	2.9612	418.7	0.173		4	^1B	2.9327	422.8	0.302
5	^1A	3.0129	411.5	0.001		5	^1A	3.0094	412.0	0.003
6	^1A	3.2551	380.9	0.009		6	^1B	3.4245	362.1	0.014
7	^1B	3.4728	357.0	0.209		7	^1B	3.4245	362.1	0.429
8	^1B	3.9285	315.6	0.478		8	^1B	3.8294	323.8	0.648
9	^1B	4.0578	305.5	0.077		9	^1B	4.0248	308.1	0.162
10	^1A	4.0976	302.6	0.000		10	^1A	4.1243	300.6	0.001
11	^1A	4.2523	291.6	0.000		11	^1B	4.2428	292.2	0.962
12	^1B	4.3962	282.0	0.787		12	^1A	4.2428	292.2	0.000
13	^1A	4.4529	278.4	0.000		13	^1A	4.4492	278.7	0.000
14	^1A	4.6273	267.9	0.000		14	^1A	4.6382	267.3	0.000
15	^1A	4.7085	263.3	0.002		15	^1A	4.7323	262.0	0.002
16	^1B	4.7819	259.3	0.174		16	^1B	4.7712	259.9	0.209
17	^1A	4.7994	258.3	0.007		17	^1A	4.8074	257.9	0.019

D. (C=C)TTP^{2+}

Gas						**CH_2Cl_2**				
	symm	eV	nm	f			symm	eV	nm	f
1	^{1}A	1.1130	1113.9	0.108		1	^{1}A	1.1150	1112.0	0.104
2		1.4454	857.8	0.069		2		1.4702	843.3	0.075
3		1.8132	683.8	0.004		3		2.2285	556.4	0.126
4		1.8688	663.5	0.026		4		2.2806	543.7	0.064
5		2.0115	616.4	0.054		5		2.3258	533.1	0.108
6		2.0705	598.8	0.014		6		2.3429	529.2	0.064
7		2.0880	593.8	0.181		7		2.3770	521.6	0.070
8		2.0996	590.5	0.063		8		2.5330	489.5	0.210
9		2.1343	580.9	0.008		9		2.5506	486.1	0.256
10		2.1383	579.8	0.031		10		2.5918	478.4	0.148
11		2.1685	571.8	0.007		11		2.5979	477.3	0.019
12		2.1851	567.4	0.041		12		2.6078	475.4	0.017
13		2.2085	561.4	0.010		13		2.6136	474.4	0.008
14		2.3068	537.5	0.030		14		2.6280	471.8	0.041
15		2.3450	528.7	0.014		15		2.6501	467.8	0.005
16		2.3852	519.8	0.003		16		2.6956	460.0	0.073
17		2.4729	501.4	0.013		17		2.8401	436.6	0.001
18		2.5110	493.8	0.085		18		2.8598	433.5	0.001
19		2.5295	490.2	0.019		19		2.9537	419.8	0.010
20		2.6024	476.4	0.014		20		2.9839	415.5	0.012
21		3.1370	395.2	0.086		21		3.1270	396.5	0.304
22		3.1445	394.3	0.180		22		3.1543	393.1	0.082
23		3.2521	381.3	0.311		23		3.2818	377.8	0.270
24		3.6495	339.7	0.354		24		3.5584	348.4	0.451
25		3.6750	337.4	1.033		25		3.6167	342.8	0.008
26		3.6869	336.3	0.010		26		3.7266	332.7	1.339
27		3.8146	325.0	0.012		27		3.8113	325.3	0.054

28		3.8556	321.6	0.003		28		3.9495	313.9	0.020
29		3.8694	320.4	0.011		29		4.0933	302.9	0.001
30		3.9753	311.9	0.093		30		4.1623	297.9	0.019
31		3.9809	311.5	0.023		31		4.1770	296.8	0.002
32		3.9981	310.1	0.009		32		4.2232	293.6	0.016
33		4.0289	307.7	0.013		33		4.2750	290.0	0.001
34		4.0493	306.2	0.005		34		4.2943	288.7	0.010
35		4.0806	303.8	0.006		35		4.3218	286.9	0.002
36		4.0939	302.9	0.006		36		4.3651	284.0	0.003
37		4.1314	300.1	0.009		37		4.5414	273.0	0.005
38		4.1390	299.6	0.002		38		4.5552	272.2	0.016
39		4.1469	299.0	0.001		39		4.5579	272.0	0.021
40		4.1498	298.8	0.021		40		4.5614	271.8	0.007

E. (C=C)TTP^{0}

Gas						**CH_2Cl_2**				
	symm	eV	nm	f			symm	eV	nm	f
1	^{1}A	0.7767	1596.2	0.001		1	^{1}A	0.7967	1556.3	0.002
2		1.6635	745.3	0.029		2		1.6598	747.0	0.049
3		2.4559	504.8	0.195		3		2.4506	505.9	0.347
4		2.7500	450.9	0.002		4		2.8077	441.6	0.004
5		2.8845	429.8	0.145		5		2.8795	430.6	0.309
6		2.9627	418.5	0.075		6		3.0565	405.6	0.036
7		2.9753	416.7	0.006		7		3.1294	396.2	0.078
8		3.0372	408.2	0.040		8		3.1325	395.8	0.026
9		3.0408	407.7	0.000		9		3.1618	392.1	0.276
10		3.0524	406.2	0.033		10		3.2093	386.3	0.024
11		3.0704	403.8	0.024		11		3.2138	385.8	0.007
12		3.0978	400.2	0.003		12		3.2187	385.2	0.001

13		3.1685	391.3	0.057		13		3.2264	384.3	0.343
14		3.2677	379.4	0.286		14		3.2811	377.9	0.010
15		3.4007	364.6	0.001		15		3.4753	356.8	0.000
16		3.5889	345.5	0.442		16		3.5216	352.1	0.002
17		3.5948	344.9	0.018		17		3.5244	351.8	0.007
18		3.6114	343.3	0.003		18		3.5301	351.2	0.027
19		3.6807	336.9	0.003		19		3.5804	346.3	0.484
20		3.6833	336.6	0.037		20		3.7461	331.0	0.241
21		3.7592	329.8	0.000		21		3.8526	321.8	0.232
22		3.7889	327.2	0.006		22		3.8621	321.0	0.000
23		3.8158	324.9	0.233		23		3.8925	318.5	0.003
24		3.8514	321.9	0.001		24		3.8999	317.9	0.152
25		3.8578	321.4	0.014		25		3.9234	316.0	0.001
26		3.8984	318.0	0.000		26		3.9392	314.8	0.079
27		3.9230	316.1	0.061		27		3.9478	314.1	0.586
28		3.9515	313.8	0.003		28		3.9873	310.9	0.006
29		3.9583	313.2	0.174		29		4.0166	308.7	0.001
30		3.9782	311.7	0.306		30		4.0217	308.3	0.001

Table S3. Orbital Contributions to Electronic Transitions in (C=C)TTP^{2+} Determined using Gaussian '09: Gas Phase and CH_2Cl_2 solution.

A. (C=C)TTP^{2+} in CH_2Cl_2

HOMO is 181 and LUMO is 182				
		eV	nm	f
1	**^{1}A**	**1.1150**	**1112.0**	**0.104**
		181	->182	0.69482
2		**1.4702**	**843.3**	**0.075**
		180	->182	0.161
		181	->183	0.67831
3		**2.2285**	**556.4**	**0.126**
		176	->182	0.44068
		179	->182	0.43466
		180	->182	-0.18431
		180	->183	0.23802
4		**2.2806**	**543.7**	**0.064**
		176	->183	-0.11795
		178	->182	-0.32903
		179	->182	0.28486
		180	->182	0.52052
5		**2.3258**	**533.1**	**0.108**
		176	->182	-0.2225
		177	->182	0.20754
		178	->182	0.53022
		179	->182	0.31087
		180	->182	0.13158
6		**2.3429**	**529.2**	**0.064**
		171	->183	0.11302
		176	->182	0.39703
		176	->183	-0.16475
		178	->182	0.26137
		179	->182	-0.31839
		179	->183	-0.1148
		180	->182	0.28938
		180	->183	0.15489
7		**2.3770**	**521.6**	**0.070**
		177	->182	0.66486

		178	->182	-0.17693
		179	->182	-0.13499
8		**2.5330**	**489.5**	**0.210**
		176	->183	0.13292
		177	->183	0.13981
		179	->183	0.6377
		180	->182	0.13582
9		**2.5506**	**486.1**	**0.256**
		171	->182	-0.21169
		175	->182	-0.17848
		176	->182	-0.21396
		176	->183	-0.1502
		177	->183	-0.10849
		178	->183	-0.27934
		180	->183	0.48967
10		**2.5918**	**478.4**	**0.148**
		171	->182	-0.21739
		174	->182	-0.24594
		175	->182	0.26084
		176	->182	-0.14462
		177	->183	0.12765
		178	->183	0.47381
		180	->183	0.21849
14		**2.6280**	**471.8**	**0.041**
		171	->182	-0.14437
		172	->182	-0.41245
		175	->182	-0.19505
		176	->183	0.45281
		179	->183	-0.1776
16		**2.6956**	**460.0**	**0.073**
		171	->183	0.11323
		172	->182	0.42443
		173	->182	-0.22769
		174	->182	-0.21607
		176	->183	0.36541
		177	->183	-0.16002
		180	->182	0.11465
		181	->183	-0.10422
21		**3.1270**	**396.5**	**0.304**
		171	->182	0.48637
		172	->183	0.27719

		173	->183	-0.1079
		180	->183	0.24188
		181	->185	-0.26417
22		**3.1543**	**393.1**	**0.082**
		181	->184	0.68764
23		**3.2818**	**377.8**	**0.270**
		170	->182	-0.26878
		171	->183	0.63115
		180	->182	-0.10822
24		**3.5584**	**348.4**	**0.451**
		170	->182	0.6389
		171	->183	0.23606
		180	->182	-0.11723
26		**3.7266**	**332.7**	**1.339**
		170	->183	0.24307
		171	->182	0.19535
		180	->183	0.15076
		181	->185	0.58776
27		**3.8113**	**325.3**	**0.054**
		170	->183	0.65556
		181	->185	-0.25272

B. (C=C)TTP^{2+} in the gas phase.

HOMO is 181 and LUMO is 182				
		eV	nm	f
1	**^{1}A**	**1.1130**	**1113.9**	**0.108**
		174	->182	0.10808
		181	->182	0.68832
2		**1.4454**	**857.8**	**0.069**
		172	->182	-0.13456
		177	->182	-0.11685
		181	->183	0.6752
5		**2.0115**	**616.4**	**0.054**
		174	->182	0.11677
		177	->182	0.11078
		178	->182	0.66316
		179	->182	-0.1394

7		**2.0880**	**593.8**	**0.181**
		173	->182	0.10009
		174	->182	-0.37486
		175	->182	0.14228
		176	->182	0.40925
		177	->182	-0.24088
		178	->182	0.1464
		180	->183	0.1919
		181	->182	0.11098
12		**2.1851**	**567.4**	**0.041**
		173	->182	0.11131
		174	->182	0.22541
		175	->182	-0.30705
		176	->182	0.34235
		179	->183	0.44188
18		**2.5110**	**493.8**	**0.085**
		171	->183	0.2568
		172	->182	0.60731
		173	->183	0.16189
		181	->183	0.11732
21		**3.1370**	**395.2**	**0.086**
		171	->182	-0.13399
		172	->183	-0.11388
		181	->184	0.6611
		181	->185	-0.10128
22		**3.1445**	**394.3**	**0.180**
		171	->182	0.4109
		172	->183	0.34935
		174	->185	0.10283
		181	->184	0.20877
		181	->185	0.35189
23		**3.2521**	**381.3**	**0.311**
		170	->182	0.28701
		171	->183	0.59218
		172	->182	-0.19145
		181	->183	-0.10294
24		**3.6495**	**339.7**	**0.354**
		170	->182	0.6028
		171	->183	-0.21315
		172	->182	0.1396
		179	->184	0.12388

		180	->184	-0.14183
25		**3.6750**	**337.4**	**1.033**
		171	->182	-0.21687
		172	->183	-0.20184
		178	->184	0.27214
		181	->185	0.54024
30		**3.9753**	**311.9**	**0.093**
		169	->183	-0.15477
		170	->183	-0.17288
		171	->182	0.10877
		172	->183	0.10562
		174	->184	0.11165
		177	->184	0.18517
		178	->184	0.55529
		179	->184	-0.10561
		181	->185	-0.1655

Table S4. Emission Excitation Energies Determined using Gaussian '09: Gas Phase.

A. Ruffled (C=C)porphine^{2+}

1st excited state						2nd excited state				
	symm	eV	nm	f			symm	eV	nm	f
1	$^1B_2$	0.593	2089.3	0.0008		1	$^1B_2$	0.702	1765.2	0.0010
2	$^1B_1$	1.131	1096.6	0.0037		2	$^1B_1$	1.108	1118.6	0.0040
3	$^1B_1$	2.243	552.9	0.0458		3	$^1B_1$	2.266	547.1	0.0298
4	$^1B_2$	2.334	531.2	0.0073		4	$^1B_2$	2.321	534.3	0.0030
5	$^1B_2$	3.005	412.7	0.1845		5	$^1B_2$	3.021	410.5	0.2163
6	$^1A_1$	3.113	398.2	0.0023		6	$^1A_1$	3.071	403.8	0.0030
7	$^1B_1$	3.178	390.1	0.1179		7	$^1B_1$	3.126	396.6	0.1595
8	$^1A_2$	3.523	352.0	0.0000		8	$^1A_2$	3.532	351.1	0.0000
9	$^1B_1$	3.642	340.4	0.5409		9	$^1B_1$	3.634	341.2	0.5211
10	$^1B_2$	3.889	318.8	0.0285		10	$^1B_2$	3.746	331.0	0.0435
11	$^1A_2$	3.907	317.3	0.0000		11	$^1A_1$	3.912	316.9	0.0029
12	$^1A_1$	4.031	307.6	0.0027		12	$^1A_2$	3.995	310.3	0.0000
13	$^1A_1$	4.163	297.8	0.0033		13	$^1A_1$	4.161	298.0	0.0026
14	$^1B_2$	4.208	294.7	1.2818		14	$^1B_2$	4.204	294.9	1.1968
15	$^1A_2$	4.237	292.6	0.0000		15	$^1A_2$	4.239	292.5	0.0000
16	$^1A_2$	4.440	279.2	0.0000		16	$^1A_2$	4.348	285.2	0.0000
17	$^1B_1$	4.744	261.3	0.2209		17	$^1A_1$	4.693	264.2	0.0007
18	$^1A_1$	4.772	259.8	0.0000		18	$^1A_2$	4.768	260.1	0.0000
19	$^1A_1$	4.831	256.6	0.0006		19	$^1B_1$	4.777	259.5	0.1982
20	$^1A_2$	4.856	255.3	0.0000		20	$^1A_1$	4.817	257.4	0.0005
21	$^1A_1$	5.116	242.4	0.0185		21	$^1A_1$	5.075	244.3	0.0326
22	$^1B_2$	5.147	240.9	0.0075		22	$^1A_2$	5.123	242.0	0.0000
23	$^1B_1$	5.161	240.3	0.0337		23	$^1B_2$	5.134	241.5	0.0179
24	$^1A_2$	5.196	238.6	0.0000		24	$^1B_1$	5.180	239.4	0.0359

25	$^1B_2$	5.584	222.0	0.0024		25	$^1B_2$	5.602	221.3	0.0104
26	$^1B_2$	5.630	220.2	0.1184		26	$^1A_2$	5.665	218.9	0.0000
27	$^1A_1$	5.687	218.0	0.0384		27	$^1B_2$	5.683	218.2	0.1023
28	$^1A_2$	5.813	213.3	0.0000		28	$^1A_1$	5.712	217.1	0.0392
29	$^1A_2$	5.869	211.3	0.0000		29	$^1B_1$	5.828	212.8	0.0269
30	$^1A_2$	5.939	208.8	0.0000		30	$^1A_2$	5.918	209.5	0.0000
31	$^1B_2$	5.939	208.8	0.3952		31	$^1A_2$	5.922	209.4	0.0000
32	$^1B_1$	5.958	208.1	0.0444		32	$^1B_1$	5.955	208.2	0.0055
33	$^1B_1$	6.014	206.2	0.0045		33	$^1B_2$	5.961	208.0	0.3710
34	$^1B_1$	6.040	205.3	0.0066		34	$^1B_1$	6.072	204.2	0.0691
35	$^1B_1$	6.173	200.9	0.1819		35	$^1B_1$	6.101	203.2	0.0223
36	$^1B_1$	6.204	199.9	0.0804		36	$^1B_1$	6.133	202.2	0.1836
37	$^1A_1$	6.231	199.0	0.0338		37	$^1A_1$	6.162	201.2	0.0419
38	$^1A_2$	6.253	198.3	0.0000		38	$^1B_2$	6.295	197.0	0.0002
39	$^1B_1$	6.263	198.0	0.0019		39	$^1A_2$	6.313	196.4	0.0000
40	$^1B_2$	6.273	197.7	0.0000		40	$^1B_1$	6.374	194.5	0.0012
41	$^1A_2$	6.334	195.8	0.0000		41	$^1B_2$	6.389	194.1	0.0108
42	$^1B_1$	6.355	195.1	0.0000		42	$^1B_1$	6.402	193.7	0.0014
43	$^1A_1$	6.416	193.3	0.0009		43	$^1A_2$	6.402	193.7	0.0000
44	$^1B_2$	6.478	191.4	0.0558		44	$^1A_1$	6.448	192.3	0.0013
45	$^1B_1$	6.486	191.2	0.3700		45	$^1B_1$	6.464	191.8	0.3329
46	$^1A_1$	6.513	190.4	0.0159		46	$^1A_1$	6.512	190.4	0.0216
47	$^1B_2$	6.582	188.4	0.0387		47	$^1B_2$	6.537	189.7	0.0583
48	$^1A_2$	6.605	187.7	0.0000		48	$^1B_1$	6.603	187.8	0.0280
49	$^1B_2$	6.671	185.9	0.0133		49	$^1B_2$	6.642	186.7	0.0088
50	$^1B_1$	6.708	184.8	0.0136		50	$^1B_1$	6.643	186.6	0.0006
51	$^1A_1$	6.720	184.5	0.0007		51	$^1A_2$	6.676	185.7	0.0000
52	$^1A_1$	6.731	184.2	0.0002		52	$^1B_2$	6.700	185.0	0.0134
53	$^1B_2$	6.739	184.0	0.0034		53	$^1A_1$	6.747	183.8	0.0001
54	$^1B_1$	6.753	183.6	0.0013		54	$^1B_2$	6.749	183.7	0.0043

55	$^1A_1$	6.795	182.5	0.0090		55	$^1A_2$	6.772	183.1	0.0000
56	$^1B_2$	6.812	182.0	0.0059		56	$^1A_1$	6.774	183.0	0.0125
57	$^1B_2$	6.819	181.8	0.0000		57	$^1A_1$	6.846	181.1	0.0043
58	$^1A_2$	6.872	180.4	0.0000		58	$^1B_2$	6.908	179.5	0.0001
59	$^1A_1$	6.911	179.4	0.0012		59	$^1A_1$	6.921	179.1	0.0049
60	$^1A_1$	6.930	178.9	0.0181		60	$^1B_1$	6.924	179.1	0.0003

3rd excited state						**4th excited state**				
	symm	eV	nm	f			symm	eV	nm	f
1	$^1B_2$	1.169	1061.0	0.0046		1	$^1B_2$	1.247	994.1	0.0057
2	$^1B_1$	1.609	770.6	0.0040		2	$^1B_1$	1.653	750.1	0.0046
3	$^1B_1$	2.306	537.7	0.0594		3	$^1B_1$	2.354	526.7	0.0533
4	$^1B_2$	2.382	520.6	0.0000		4	$^1B_2$	2.385	519.9	0.0004
5	$^1B_2$	3.183	389.5	0.3698		5	$^1B_1$	3.184	389.4	0.1608
6	$^1B_1$	3.197	387.9	0.1460		6	$^1B_2$	3.188	388.9	0.3797
7	$^1A_2$	3.571	347.2	0.0000		7	$^1A_2$	3.562	348.1	0.0000
8	$^1A_1$	3.572	347.1	0.0032		8	$^1A_1$	3.564	347.9	0.0035
9	$^1B_1$	3.677	337.2	0.4758		9	$^1B_1$	3.644	340.3	0.4963
10	$^1B_2$	3.851	321.9	0.0625		10	$^1B_2$	3.803	326.0	0.0650
11	$^1A_1$	4.002	309.8	0.0041		11	$^1A_1$	3.954	313.5	0.0046
12	$^1A_1$	4.144	299.2	0.0038		12	$^1A_1$	4.152	298.6	0.0044
13	$^1A_2$	4.221	293.8	0.0000		13	$^1A_2$	4.240	292.4	0.0000
14	$^1A_2$	4.322	286.9	0.0000		14	$^1A_2$	4.314	287.4	0.0000
15	$^1B_2$	4.405	281.4	0.9889		15	$^1B_2$	4.414	280.9	0.9258
16	$^1A_2$	4.499	275.6	0.0000		16	$^1A_2$	4.571	271.2	0.0000
17	$^1B_1$	4.683	264.8	0.2611		17	$^1B_1$	4.697	264.0	0.2044
18	$^1A_2$	4.780	259.4	0.0000		18	$^1A_1$	4.734	261.9	0.0001
19	$^1A_1$	4.783	259.2	0.0000		19	$^1A_2$	4.754	260.8	0.0000
20	$^1A_1$	4.802	258.2	0.0001		20	$^1A_1$	4.766	260.1	0.0001
21	$^1A_1$	5.109	242.7	0.0281		21	$^1A_2$	5.101	243.1	0.0000

22	$^1A_2$	5.151	240.7	0.0000		22	$^1A_1$	5.107	242.8	0.0384
23	$^1B_2$	5.219	237.6	0.0783		23	$^1B_2$	5.203	238.3	0.1229
24	$^1B_1$	5.594	221.7	0.0085		24	$^1B_1$	5.619	220.6	0.0054
25	$^1B_2$	5.615	220.8	0.0129		25	$^1B_2$	5.620	220.6	0.0112
26	$^1A_1$	5.760	215.2	0.0705		26	$^1A_2$	5.672	218.6	0.0000
27	$^1A_2$	5.772	214.8	0.0000		27	$^1A_1$	5.807	213.5	0.0709
28	$^1B_2$	5.830	212.7	0.0001		28	$^1B_1$	5.823	212.9	0.0321
29	$^1B_1$	5.914	209.6	0.0436		29	$^1B_2$	5.843	212.2	0.0007
30	$^1B_1$	5.994	206.9	0.0181		30	$^1B_1$	5.968	207.7	0.0357
31	$^1A_2$	6.004	206.5	0.0000		31	$^1A_2$	5.998	206.7	0.0000
32	$^1B_1$	6.102	203.2	0.1953		32	$^1B_1$	6.072	204.2	0.2239
33	$^1B_1$	6.193	200.2	0.0097		33	$^1B_1$	6.178	200.7	0.0348
34	$^1B_1$	6.234	198.9	0.0793		34	$^1A_2$	6.263	198.0	0.0000
35	$^1A_2$	6.272	197.7	0.0000		35	$^1B_2$	6.282	197.4	0.4767
36	$^1B_2$	6.278	197.5	0.5122		36	$^1B_1$	6.302	196.8	0.0261
37	$^1A_2$	6.293	197.0	0.0000		37	$^1A_2$	6.305	196.7	0.0000
38	$^1B_1$	6.308	196.6	0.0044		38	$^1B_1$	6.333	195.8	0.0003
39	$^1A_2$	6.334	195.7	0.0000		39	$^1A_2$	6.348	195.3	0.0000
40	$^1B_1$	6.346	195.4	0.0000		40	$^1B_2$	6.365	194.8	0.0115
41	$^1A_1$	6.415	193.3	0.0003		41	$^1B_1$	6.382	194.3	0.0022
42	$^1B_2$	6.426	193.0	0.0000		42	$^1A_1$	6.447	192.3	0.0003
43	$^1B_2$	6.503	190.7	0.0001		43	$^1B_2$	6.532	189.8	0.0006
44	$^1B_2$	6.538	189.6	0.0441		44	$^1A_1$	6.543	189.5	0.0257
45	$^1A_1$	6.554	189.2	0.0238		45	$^1B_2$	6.558	189.1	0.0415
46	$^1B_1$	6.608	187.6	0.0405		46	$^1B_1$	6.569	188.8	0.0343
47	$^1B_2$	6.692	185.3	0.0199		47	$^1B_2$	6.682	185.6	0.0088
48	$^1A_1$	6.708	184.8	0.0000		48	$^1A_1$	6.707	184.9	0.0002
49	$^1A_1$	6.715	184.6	0.0063		49	$^1A_1$	6.713	184.7	0.0072
50	$^1B_2$	6.719	184.5	0.0056		50	$^1B_2$	6.734	184.1	0.0210
51	$^1A_2$	6.731	184.2	0.0000		51	$^1A_2$	6.772	183.1	0.0000

52	$^1A_2$	6.778	182.9	0.0000		52	$^1A_2$	6.777	182.9	0.0000
53	$^1A_1$	6.824	181.7	0.0449		53	$^1A_1$	6.829	181.6	0.0427
54	$^1B_1$	6.853	180.9	0.1286		54	$^1B_1$	6.843	181.2	0.1589
55	$^1A_2$	6.857	180.8	0.0000		55	$^1B_2$	6.865	180.6	0.0015
56	$^1B_1$	6.892	179.9	0.1302		56	$^1A_2$	6.867	180.6	0.0000
57	$^1A_1$	6.904	179.6	0.0000		57	$^1B_1$	6.891	179.9	0.0900
58	$^1B_1$	6.905	179.6	0.0020		58	$^1B_1$	6.905	179.6	0.0017
59	$^1B_2$	6.933	178.8	0.0000		59	$^1A_1$	6.912	179.4	0.0009
60	$^1A_1$	7.025	176.5	0.0019		60	$^1A_1$	7.038	176.2	0.0022

B. (C=C)TTP^{2+}

1st excited state						**2nd excited state**				
	symm	eV	nm	f			symm	eV	nm	f
1	^1A	0.677	1831.5	0.0314		1	^1A	1.113	1113.94	0.1077
2		1.152	1076.2	0.0436		2		1.445	857.79	0.0692
3		1.721	720.5	0.0032		3		1.813	683.8	0.0037
4		1.779	697.0	0.0082		4		1.869	663.46	0.0258
5		1.845	672.1	0.2135		5		2.012	616.38	0.0536
6		1.914	647.9	0.0813		6		2.071	598.81	0.0139
7		2.006	618.0	0.0073		7		2.088	593.8	0.1809
8		2.038	608.5	0.0007		8		2.100	590.51	0.0628
9		2.068	599.7	0.0004		9		2.134	580.92	0.0077
10		2.083	595.1	0.0014		10		2.138	579.83	0.0314
11		2.119	585.2	0.1022		11		2.169	571.76	0.007
12		2.177	569.5	0.0101		12		2.185	567.41	0.0407
13		2.205	562.3	0.0753		13		2.209	561.4	0.0101
14		2.225	557.3	0.0148		14		2.307	537.48	0.0298
15		2.350	527.7	0.0240		15		2.345	528.71	0.0135
16		2.425	511.2	0.0041		16		2.385	519.81	0.003

17		2.439	508.4	0.1329		17		2.473	501.38	0.0133
18		2.477	500.5	0.0075		18		2.511	493.77	0.0848
19		2.526	490.9	0.0066		19		2.530	490.15	0.0185
20		2.572	482.0	0.0005		20		2.602	476.43	0.0138
21		2.900	427.5	0.0431		21		3.137	395.23	0.0858
22		2.974	416.9	0.0580		22		3.145	394.29	0.1797
23		3.234	383.4	0.2339		23		3.252	381.24	0.3109
24		3.609	343.5	0.3612		24		3.650	339.73	0.3537
25		3.629	341.7	0.0815		25		3.675	337.37	1.0335
26		3.639	340.7	1.3313		26		3.687	336.29	0.0102
27		3.826	324.1	0.0029		27		3.815	325.02	0.0122
28		3.852	321.9	0.0142		28		3.856	321.57	0.0026
29		3.896	318.3	0.0036		29		3.869	320.42	0.0106
30		3.920	316.3	0.0194		30		3.981	311.45	0.0929
31		3.926	315.8	0.0175		31		3.998	310.11	0.0234
32		4.015	308.8	0.0489		32		4.029	307.73	0.0086
33		4.017	308.7	0.0588		33		4.081	303.84	0.0137
34		4.056	305.7	0.0021		34		4.094	302.85	0.005
35		4.081	303.8	0.0141		35		4.131	300.1	0.0057
36		4.135	299.9	0.0018		36		4.147	298.98	0.0066
37		4.176	296.9	0.0019		37		4.150	298.77	0.0092
38		4.210	294.5	0.0088		38		4.196	295.49	0.0015
39		4.227	293.3	0.0018		39		4.220	293.77	0.0007
40		4.272	290.2	0.0105		40		4.326	286.63	0.0225
41		4.310	287.7	0.0005		41		4.354	284.73	0.0169
42		4.322	286.9	0.0065		42		4.355	284.72	0.0046
43		4.329	286.4	0.0337		43		4.369	283.78	0.0116
44		4.359	284.4	0.0243		44		4.391	282.36	0.0031
45		4.368	283.9	0.0005		45		4.401	281.74	0.0026
46		4.396	282.1	0.0260		46		4.412	281.02	0.0409

47		4.409	281.2	0.0205		47		4.444	279	0.0006
48		4.440	279.2	0.0021		48		4.505	275.21	0.0599
49		4.485	276.4	0.0254		49		4.510	274.9	0.0082
50		4.499	275.6	0.1137		50		4.513	274.72	0.0797
51		4.504	275.3	0.0164		51		4.553	272.3	0.0038
52		4.510	274.9	0.0372		52		4.573	271.12	0.0027
53		4.540	273.1	0.0242		53		4.595	269.85	0.002
54		4.553	272.3	0.1301		54		4.619	268.45	0.0044
55		4.583	270.5	0.0195		55		4.632	267.7	0.0023
56		4.599	269.6	0.0006		56		4.647	266.8	0.0218
57		4.613	268.8	0.0549		57		4.670	265.49	0.004
58		4.626	268.0	0.0081		58		4.674	265.25	0.0011
59		4.652	266.5	0.0005		59		4.693	264.21	0.0026
60		4.663	265.9	0.0039		60		4.714	263.04	0.0622

3rd excited state						**4th excited state**				
	symm	eV	nm	f			symm	eV	nm	f
1	^{1}A	1.054	1176.0	0.0826		1	^{1}A	0.831	1493.0	0.0521
2		1.306	949.3	0.0002		2		1.127	1100.5	0.0371
3		1.497	828.3	0.0413		3		1.777	697.9	0.0050
4		1.694	731.9	0.0001		4		1.783	695.5	0.0021
5		1.775	698.7	0.0463		5		1.949	636.0	0.1332
6		1.848	670.8	0.0323		6		1.972	628.7	0.1684
7		1.906	650.6	0.1292		7		1.978	626.7	0.0477
8		1.981	625.8	0.0270		8		2.006	618.1	0.0375
9		1.990	623.0	0.0045		9		2.047	605.8	0.0462
10		2.002	619.5	0.0198		10		2.110	587.7	0.0016
11		2.054	603.7	0.0033		11		2.124	583.7	0.0092
12		2.182	568.2	0.0613		12		2.131	581.7	0.0001
13		2.207	561.9	0.0046		13		2.173	570.7	0.0022

14		2.313	536.0	0.0383		14		2.174	570.3	0.0014
15		2.347	528.2	0.0192		15		2.218	559.1	0.0303
16		2.421	512.0	0.0013		16		2.262	548.1	0.0003
17		2.452	505.6	0.0463		17		2.458	504.4	0.0231
18		2.455	505.1	0.0673		18		2.468	502.3	0.0017
19		2.467	502.6	0.0019		19		2.469	502.1	0.0532
20		2.574	481.6	0.0034		20		2.535	489.0	0.0344
21		3.109	398.8	0.2744		21		2.870	432.0	0.0527
22		3.221	385.0	0.0628		22		2.999	413.4	0.0608
23		3.264	379.8	0.2493		23		3.172	390.8	0.3591
24		3.436	360.9	0.0001		24		3.597	344.7	1.2541
25		3.593	345.1	0.0112		25		3.624	342.1	0.3827
26		3.608	343.7	0.4428		26		3.656	339.2	0.0001
27		3.738	331.7	0.8697		27		3.729	332.5	0.0048
28		3.896	318.2	0.0001		28		3.755	330.2	0.0373
29		3.909	317.2	0.0082		29		3.761	329.7	0.0075
30		3.924	316.0	0.0330		30		3.861	321.1	0.0307
31		3.947	314.1	0.0025		31		3.925	315.9	0.0011
32		3.989	310.9	0.2159		32		3.936	315.0	0.0964
33		4.017	308.7	0.0167		33		3.948	314.0	0.0007
34		4.035	307.3	0.0297		34		3.998	310.1	0.0005
35		4.048	306.3	0.0047		35		4.059	305.5	0.0362
36		4.109	301.7	0.0141		36		4.061	305.3	0.0095
37		4.135	299.8	0.0031		37		4.102	302.3	0.0035
38		4.142	299.3	0.0009		38		4.158	298.2	0.0008
39		4.147	299.0	0.0078		39		4.163	297.8	0.0011
40		4.185	296.2	0.0307		40		4.286	289.3	0.0004
41		4.236	292.7	0.0014		41		4.304	288.1	0.0473
42		4.246	292.0	0.0002		42		4.308	287.8	0.0235
43		4.277	289.9	0.0038		43		4.319	287.1	0.0135

44		4.338	285.8	0.0053		44		4.367	283.9	0.0575
45		4.363	284.2	0.0228		45		4.375	283.4	0.0086
46		4.376	283.4	0.0239		46		4.381	283.0	0.0004
47		4.383	282.9	0.0012		47		4.390	282.4	0.0014
48		4.392	282.3	0.0012		48		4.452	278.5	0.0008
49		4.414	280.9	0.0013		49		4.488	276.3	0.0041
50		4.430	279.9	0.0025		50		4.497	275.7	0.0336
51		4.450	278.6	0.0005		51		4.499	275.6	0.0485
52		4.465	277.7	0.0041		52		4.525	274.0	0.0212
53		4.487	276.3	0.0012		53		4.554	272.3	0.2259
54		4.511	274.9	0.0071		54		4.561	271.8	0.0006
55		4.515	274.6	0.1559		55		4.586	270.3	0.0002
56		4.586	270.4	0.0011		56		4.609	269.0	0.0040
57		4.610	268.9	0.0181		57		4.622	268.2	0.0028
58		4.638	267.3	0.0391		58		4.626	268.0	0.0008
59		4.643	267.0	0.0130		59		4.643	267.0	0.0022
60		4.648	266.8	0.0031		60		4.673	265.3	0.0053

Table S5. Total Energies at B3LYP/DZVP2/aug-cc-pVDZ (Zn) Level of Theory Given in Hartrees.

Compound	**ZPE**	**E**	**H_{298K}**	**G_{298K}**
Zn(porphine)	0.273618	-1215.484509	-1215.466000	-1215.526760
planar (C=C)porphine^{2+}	0.288921	-1063.843002	-1063.826610	-1063.883540
ruffled (C=C)porphine^{2+}	0.288914	-1063.856515	-1063.839471	-1063.898099
(C=C)porphine^{0}	0.285805	-1064.386122	-1064.368602	-1064.428088
(C=C)TTP^{2+}	0.719950	-2145.150613	-2145.106040	-2145.232450
(C=C)TTP^{0}	0.717207	-2145.624536	-2145.579393	-2145.708314

Table S6. Optimized B3LYP/DZVP2/aug-cc-pVDZ (Zn) Cartesian Coordinates in Angstroms for the Various Structures.

Zn(porphine)

C	1.103858	2.870320	0.000000
C	0.684434	4.256641	0.000000
C	-0.684434	4.256641	0.000000
C	-1.103858	2.870320	0.000000
N	0.000000	2.052315	0.000000
H	1.351381	5.109069	0.000000
H	-1.351381	5.109069	0.000000
C	2.432913	2.432913	0.000000
H	3.200509	3.200509	0.000000
C	2.870320	1.103857	0.000000
C	4.256641	0.684434	0.000000
C	4.256641	-0.684434	0.000000
H	5.109069	1.351381	0.000000
C	2.870320	-1.103858	0.000000
H	5.109069	-1.351381	0.000000
C	2.432913	-2.432913	0.000000
H	3.200509	-3.200509	0.000000
C	-2.432913	2.432913	0.000000
H	-3.200509	3.200509	0.000000
C	1.103858	-2.870320	0.000000
C	0.684434	-4.256641	0.000000
C	-0.684434	-4.256641	0.000000
H	1.351381	-5.109069	0.000000
C	-1.103858	-2.870320	0.000000
H	-1.351381	-5.109069	0.000000
C	-2.870320	1.103858	0.000000
C	-4.256641	0.684434	0.000000
C	-4.256641	-0.684434	0.000000
H	-5.109069	1.351381	0.000000
C	-2.870320	-1.103857	0.000000
H	-5.109069	-1.351381	0.000000
C	-2.432913	-2.432913	0.000000
H	-3.200509	-3.200509	0.000000
N	0.000000	-2.052315	0.000000
N	-2.052315	0.000000	0.000000
N	2.052315	0.000000	0.000000
ZN	0.000000	0.000000	0.000000

planar (C=C)porphine^{2+}

C	0.000000	2.561905	1.233867
C	0.000000	3.339076	2.424006

C	0.000000	2.480721	3.489841
C	0.000000	1.165732	2.961971
N	0.000000	1.195555	1.555672
H	0.000000	4.420844	2.435845
H	0.000000	2.712239	4.546801
C	0.000000	3.167490	0.000000
H	0.000000	4.250626	0.000000
C	0.000000	2.561905	-1.233867
C	0.000000	3.339076	-2.424006
C	0.000000	2.480721	-3.489841
H	0.000000	4.420844	-2.435845
C	0.000000	1.165732	-2.961971
H	0.000000	2.712239	-4.546801
C	0.000000	0.000000	-3.687985
H	0.000000	0.000000	-4.769686
C	0.000000	0.000000	3.687985
H	0.000000	0.000000	4.769686
C	0.000000	-1.165732	-2.961971
C	0.000000	-2.480721	-3.489841
C	0.000000	-3.339076	-2.424006
H	0.000000	-2.712239	-4.546801
C	0.000000	-2.561905	-1.233867
H	0.000000	-4.420844	-2.435845
C	0.000000	-1.165732	2.961971
C	0.000000	-2.480721	3.489841
C	0.000000	-3.339076	2.424006
H	0.000000	-2.712239	4.546801
C	0.000000	-2.561905	1.233867
H	0.000000	-4.420844	2.435845
C	0.000000	-3.167490	0.000000
H	0.000000	-4.250626	0.000000
N	0.000000	-1.195555	-1.555672
N	0.000000	-1.195555	1.555672
N	0.000000	1.195555	-1.555672
C	0.000000	0.000000	-0.695580
C	0.000000	0.000000	0.695580

ruffled (C=C)porphine^{2+}

C	-1.179842	2.816845	-0.494559
C	-2.472478	3.375597	-0.285819
C	-3.231738	2.427927	0.361773
C	-2.457320	1.235498	0.475141
N	-1.184322	1.494843	-0.043958
H	-2.758648	4.382735	-0.559142
H	-4.257582	2.520143	0.693712
C	0.000000	3.463534	-0.835433

H	0.000000	4.491509	-1.174875
C	1.179842	2.816845	-0.494559
C	2.472478	3.375597	-0.285819
C	3.231738	2.427927	0.361773
H	2.758648	4.382735	-0.559142
C	2.457320	1.235498	0.475141
H	4.257582	2.520143	0.693712
C	2.989490	0.000000	0.818650
H	4.000128	0.000000	1.211334
C	-2.989490	0.000000	0.818650
H	-4.000128	0.000000	1.211334
C	2.457320	-1.235498	0.475141
C	3.231738	-2.427927	0.361773
C	2.472478	-3.375597	-0.285819
H	4.257582	-2.520143	0.693712
C	1.179842	-2.816845	-0.494559
H	2.758648	-4.382735	-0.559142
C	-2.457320	-1.235498	0.475141
C	-3.231738	-2.427927	0.361773
C	-2.472478	-3.375597	-0.285819
H	-4.257582	-2.520143	0.693712
C	-1.179842	-2.816845	-0.494559
H	-2.758648	-4.382735	-0.559142
C	0.000000	-3.463534	-0.835433
H	0.000000	-4.491509	-1.174875
N	1.184322	-1.494843	-0.043958
N	-1.184322	-1.494843	-0.043958
N	1.184322	1.494843	-0.043958
C	0.000000	-0.680137	-0.044652
C	0.000000	0.680137	-0.044652

(C=C)porphine^{0}

C	-2.691678	-1.436476	0.556420
C	-4.026519	-1.058251	0.404781
C	-4.026519	0.181114	-0.259781
C	-2.703005	0.577939	-0.461558
N	-1.870644	-0.420667	0.046714
H	-4.876205	-1.668339	0.674361
H	-4.885908	0.773931	-0.542501
C	-2.146765	-2.710224	0.869399
H	-2.788692	-3.516763	1.195029
C	-0.870412	-2.941296	0.454367
C	-0.201116	-4.201906	0.208046
C	0.957042	-3.938975	-0.448549
H	-0.617394	-5.164234	0.471201
C	1.135183	-2.503997	-0.538115

H	1.693761	-4.648659	-0.800832
C	2.315370	-1.897863	-0.825487
H	3.111138	-2.533822	-1.196673
C	-2.315370	1.897863	-0.825487
H	-3.111138	2.533822	-1.196673
C	2.703005	-0.577939	-0.461558
C	4.026519	-0.181114	-0.259781
C	4.026519	1.058251	0.404781
H	4.885908	-0.773931	-0.542501
C	2.691678	1.436476	0.556420
H	4.876205	1.668339	0.674361
C	-1.135183	2.503997	-0.538115
C	-0.957042	3.938975	-0.448549
C	0.201116	4.201906	0.208046
H	-1.693761	4.648659	-0.800832
C	0.870412	2.941296	0.454367
H	0.617394	5.164234	0.471201
C	2.146765	2.710224	0.869399
H	2.788692	3.516763	1.195029
N	1.870644	0.420667	0.046714
N	0.034146	1.905473	-0.005472
N	-0.034146	-1.905473	-0.005472
C	0.430503	0.537865	0.025596
C	-0.430503	-0.537865	0.025596

(C=C)TTP^{2+}

C	-0.927944	2.559701	0.437199
C	-1.986052	3.479345	0.197236
H	-1.955131	4.520529	0.480396
C	-2.973619	2.837113	-0.519328
H	-3.881554	3.268438	-0.912558
C	-2.602200	1.475384	-0.643827
C	-3.371145	0.365403	-1.034662
C	-2.858808	-0.875602	-0.617065
C	-3.569691	-2.076342	-0.363635
H	-4.597749	-2.250354	-0.645618
C	-2.737892	-2.915894	0.346594
H	-2.961773	-3.907794	0.709426
C	-1.468260	-2.287645	0.481115
C	-0.302287	-2.958375	0.888248
C	0.982872	-2.559984	0.493365
C	2.088372	-3.448870	0.373924
H	2.093711	-4.459663	0.751577
C	3.078731	-2.825386	-0.350970
H	4.019409	-3.247354	-0.670156
C	2.675742	-1.483204	-0.572849

C	3.454761	-0.379413	-0.952294
C	2.929134	0.862281	-0.555259
C	3.659159	2.030648	-0.217635
H	4.707461	2.177903	-0.432478
C	2.821804	2.858080	0.498483
H	3.072347	3.805866	0.949635
C	1.521897	2.279223	0.521395
C	0.349148	2.956301	0.881778
C	-0.646691	0.068838	-0.091418
C	0.698870	-0.073912	-0.099979
C	-4.691450	0.457053	-1.679016
C	-5.711771	1.308496	-1.202999
H	-5.564707	1.883470	-0.294570
C	-6.948994	1.353509	-1.841044
H	-7.729957	1.993208	-1.439702
C	-7.215477	0.572785	-2.983813
C	-6.198055	-0.279272	-3.448711
H	-6.374708	-0.892412	-4.327528
C	-4.962445	-0.349147	-2.804681
H	-4.188659	-0.999665	-3.201504
C	-8.548591	0.658816	-3.684202
H	-9.371567	0.686485	-2.964659
H	-8.703798	-0.186827	-4.357065
H	-8.607994	1.576592	-4.280613
C	-0.484003	-4.263810	1.594073
C	-0.920451	-4.263963	2.930437
H	-1.097774	-3.323670	3.444565
C	-1.111648	-5.469159	3.611447
H	-1.437958	-5.446684	4.647377
C	-0.894548	-6.706903	2.980524
C	-0.482864	-6.695072	1.635795
H	-0.331986	-7.636418	1.115162
C	-0.273577	-5.495661	0.949953
H	0.016572	-5.522562	-0.096753
C	-1.084961	-8.005597	3.727539
H	-0.177268	-8.262438	4.285605
H	-1.297503	-8.831214	3.044670
H	-1.902695	-7.933473	4.448916
C	4.804628	-0.470118	-1.538328
C	5.103419	0.301699	-2.679968
H	4.334059	0.924677	-3.126702
C	6.365095	0.235955	-3.273100
H	6.564152	0.823257	-4.164715
C	7.379612	-0.578217	-2.740095
C	7.084246	-1.322430	-1.580556
H	7.861139	-1.930889	-1.126161

C	5.822140	-1.280190	-0.991698
H	5.651986	-1.824885	-0.068688
C	8.740223	-0.661972	-3.386504
H	8.908603	0.167940	-4.075710
H	8.836071	-1.593894	-3.955525
H	9.535397	-0.657313	-2.635947
C	0.434957	4.265999	1.589118
C	1.043709	5.395330	1.009129
H	1.449626	5.340370	0.003180
C	1.077839	6.609477	1.696318
H	1.532025	7.474755	1.221626
C	0.525297	6.738191	2.985055
C	-0.088402	5.607936	3.551686
H	-0.528691	5.678370	4.542075
C	-0.147828	4.393329	2.863031
H	-0.628564	3.537127	3.327319
C	0.601062	8.047153	3.733529
H	1.586095	8.164757	4.199583
H	-0.148719	8.098823	4.525829
H	0.455096	8.897236	3.061972
N	-1.325241	1.325669	-0.086268
N	-1.568283	-1.020816	-0.105831
N	1.371535	-1.337327	-0.085097
N	1.617222	1.023367	-0.111702

(C=C)TTP^{0}

C	-1.009324	2.546674	0.541429
C	-2.171543	3.408370	0.449290
H	-2.188063	4.422043	0.820048
C	-3.143436	2.774118	-0.252932
H	-4.104680	3.165239	-0.549723
C	-2.706788	1.419794	-0.509543
C	-3.423764	0.344642	-0.961968
C	-2.869976	-0.936980	-0.644676
C	-3.533384	-2.152601	-0.484230
H	-4.557581	-2.338683	-0.769149
C	-2.667914	-3.004686	0.222899
H	-2.861252	-4.023041	0.524189
C	-1.462047	-2.334823	0.445944
C	-0.247045	-2.980889	0.859227
C	1.008966	-2.549280	0.538639
C	2.170877	-3.411190	0.445005
H	2.187183	-4.425373	0.814376
C	3.142673	-2.776381	-0.256846
H	4.103480	-3.167631	-0.554810
C	2.706448	-1.421537	-0.511477

C	3.423621	-0.345793	-0.962294
C	2.869820	0.935476	-0.643258
C	3.533295	2.150851	-0.481219
H	4.557578	2.337198	-0.765620
C	2.667672	3.002283	0.226479
H	2.860985	4.020332	0.528808
C	1.461710	2.332280	0.448498
C	0.246687	2.978110	0.862156
C	-0.682161	0.064535	-0.061789
C	0.681906	-0.066578	-0.061883
C	-4.798919	0.438966	-1.513669
C	-5.850422	1.053120	-0.811874
H	-5.668101	1.454466	0.180160
C	-7.138521	1.119994	-1.355887
H	-7.932455	1.594912	-0.784782
C	-7.427077	0.571840	-2.614411
C	-6.379443	-0.060101	-3.306803
H	-6.573016	-0.501798	-4.281489
C	-5.092689	-0.128962	-2.767833
H	-4.300166	-0.619274	-3.325409
C	-8.812952	0.665225	-3.215710
H	-8.856404	1.446970	-3.983502
H	-9.559952	0.906524	-2.454732
H	-9.103889	-0.276160	-3.692194
C	-0.401894	-4.333232	1.491430
C	-0.602298	-4.447749	2.876135
H	-0.637239	-3.548394	3.484066
C	-0.754940	-5.701631	3.476943
H	-0.905724	-5.762776	4.552036
C	-0.718429	-6.882069	2.715865
C	-0.529795	-6.762477	1.330148
H	-0.506199	-7.657718	0.713858
C	-0.374823	-5.508971	0.725938
H	-0.237591	-5.440694	-0.349565
C	-0.859440	-8.237217	3.375618
H	0.080074	-8.541062	3.852403
H	-1.125359	-9.007547	2.646871
H	-1.629938	-8.222220	4.152507
C	4.798774	-0.438596	-1.514071
C	5.092660	0.135069	-2.766261
H	4.299686	0.626592	-3.322133
C	6.378611	0.067744	-3.305804
H	6.571732	0.512002	-4.279529
C	7.426814	-0.567337	-2.615895
C	7.137620	-1.123702	-1.361886
H	7.930512	-1.605126	-0.794983

C	5.849416	-1.057917	-0.816580
H	5.666877	-1.466513	0.172423
C	8.816648	-0.638124	-3.211274
H	8.816779	-1.206211	-4.148393
H	9.517123	-1.121700	-2.525531
H	9.201846	0.362076	-3.437850
C	0.401669	4.330282	1.494690
C	0.373232	5.506158	0.729485
H	0.234707	5.438039	-0.345862
C	0.528535	6.759616	1.333741
H	0.503856	7.654961	0.717649
C	0.718864	6.878996	2.719219
C	0.756689	5.698397	3.480033
H	0.908761	5.759402	4.554956
C	0.603774	4.444588	2.879182
H	0.639791	3.545123	3.486886
C	0.860567	8.233993	3.379136
H	1.119993	9.005536	2.649347
H	1.635999	8.220336	4.151157
H	-0.076648	8.535081	3.862128
N	-1.384870	1.298675	-0.026928
N	-1.586874	-1.052341	-0.095820
N	1.384589	-1.300775	-0.028511
N	1.586608	1.050342	-0.094589

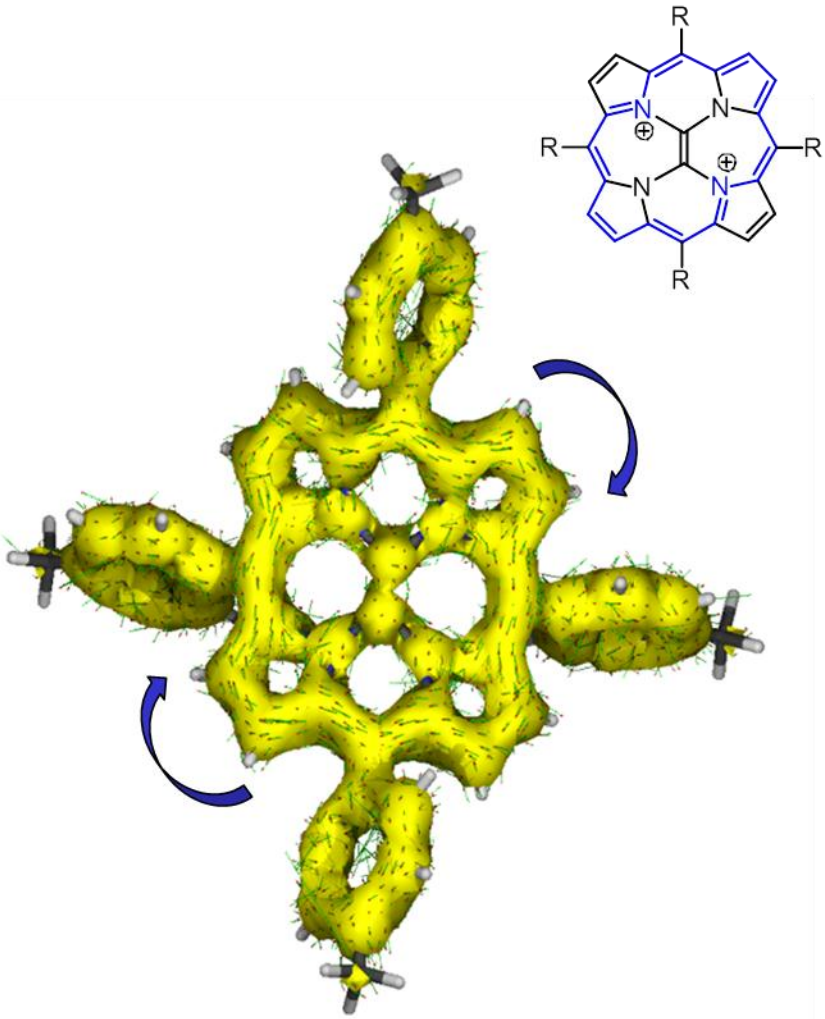


Figure S2. Anisotropy of the Induced Current Density (ACID) plot for (C=C)TTP^{2+} (ISP = 0.05).

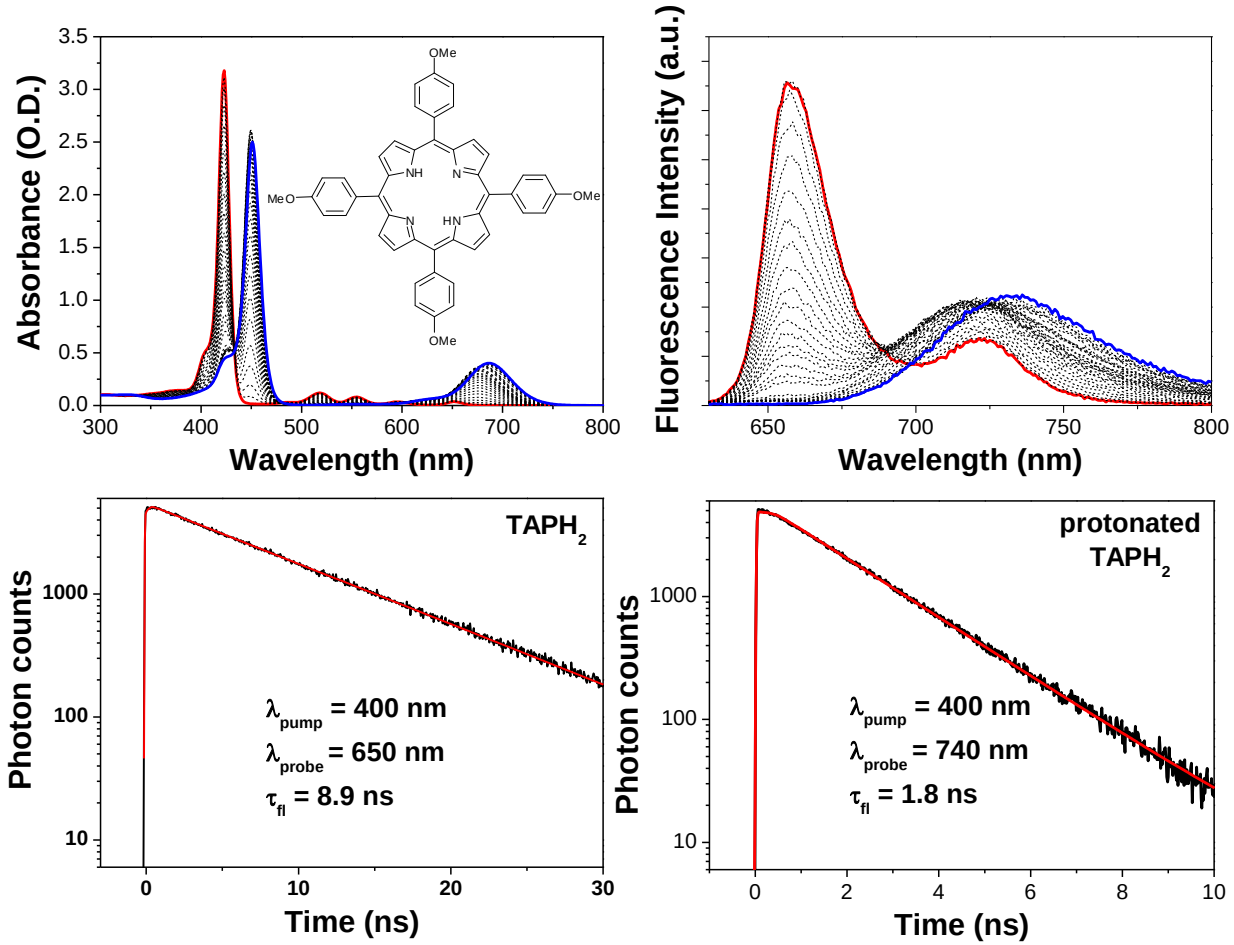


Figure S3. Absorption (top left) and fluorescence (top right) spectral change of tetramethoxyphenyl porphyrin upon protonation(red: neutral, blue: protonated form) and fluorescence decay profile of neutral form (bottom left) and protonated from (bottom right)