

Supporting information for manuscript:

The first TDDFT and MCD studies of free base triarylcorroles: A closer look into solvent-dependent UV-visible absorption

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Experimental Section

Reagents and materials. Synthesis and characterization of all corroles used in this paper have already been described in the literature.¹ N,N-dimethylformamide and DCM were purchased from Acros and were distilled over calcium hydride prior spectroscopic experiments.

Spectroscopy Measurements. UV-Vis data were obtained on Jasco-720 or Cary 17 spectrophotometers. MCD data were recorded using OLIS DCM 17 CD spectropolarimeter with a 1.4 T DeSa magnet. The MCD spectra were measured in mdeg = $[\theta]$ and converted to $\Delta\epsilon$ ($M^{-1} \text{ cm}^{-1} \text{ T}^{-1}$) using the regular conversion formula: $\Delta\epsilon = \theta / (32980 \cdot Bdc)$, where B is the magnetic field, d is the path length, and c is the concentration. Complete spectra were recorded at room temperature in parallel and anti-parallel directions with respect to the magnetic field. In all cases UV-vis spectra were recorded for samples before and after MCD experiments in order to ensure that samples were stable during experiments.

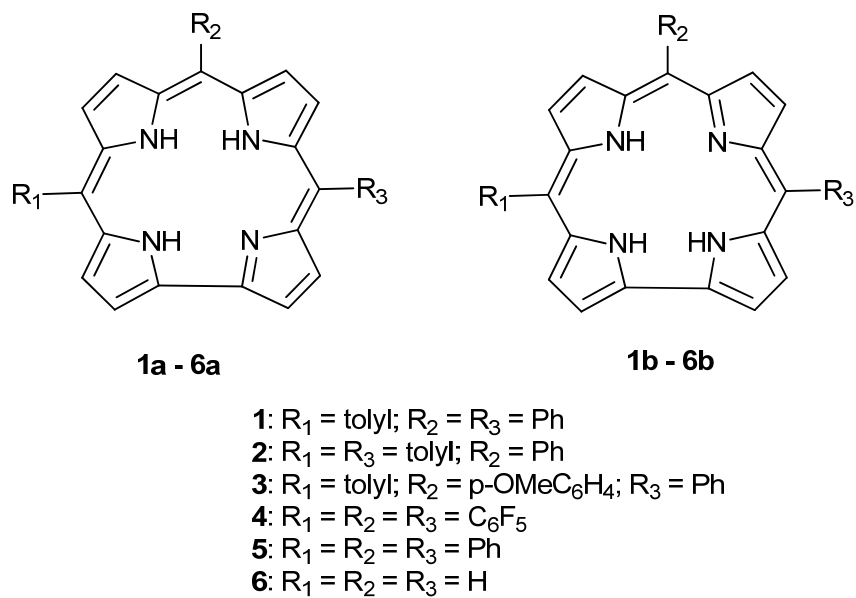
DFT-PCM and TDDFT-PCM Calculations. Calculations were carried out on **5a** and **5b** as well as the simplified tautomers **6a** and **6b** where the phenyl groups are replaced with hydrogen atoms at the three *meso* carbon positions. Geometry optimizations were conducted for both point groups using the polarized continuum model (PCM) approach² and DCM and DMF were used as solvent. Converged geometries were tested by frequency calculations in order to confirm the nature of stationary points. Geometries were not restricted in these calculations. All geometry optimizations, single-point DFT-PCM and TDDFT-PCM calculations were conducted using a pure BP86 functional.³ The first 50 states were considered in all PCM-TDDFT calculations. In all cases, 6-31G(d) basis set was used for all atoms.⁴ All calculations were performed using Gaussian 09 software.⁵ TDDFT predicted UV-vis spectra profiles were modeled using

GaussView software⁶ and 800 cm⁻¹ bandwidth for all bands. Molecular orbital analysis was conducted using the QMForge program.

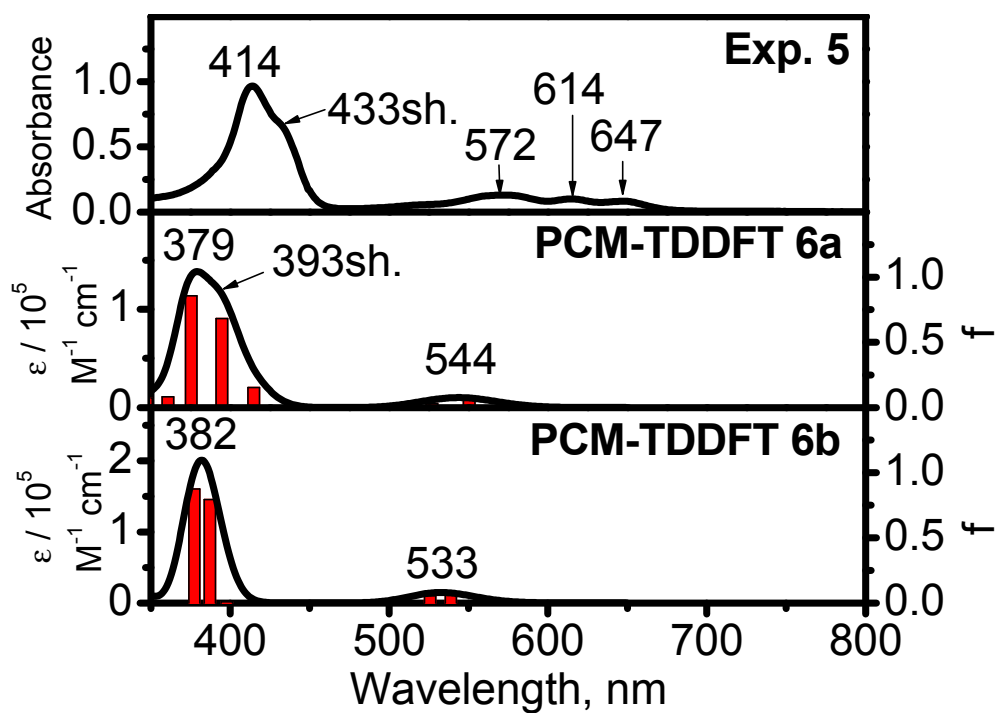
References

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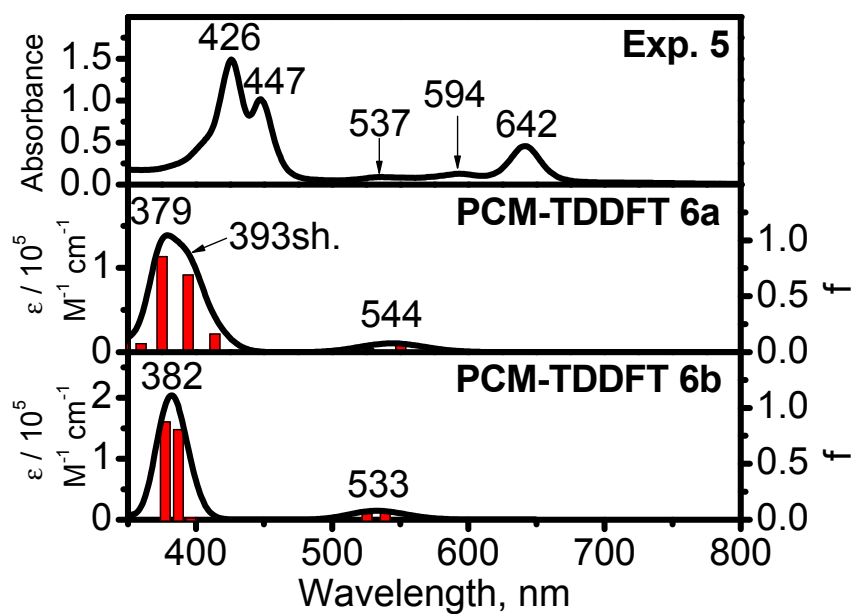
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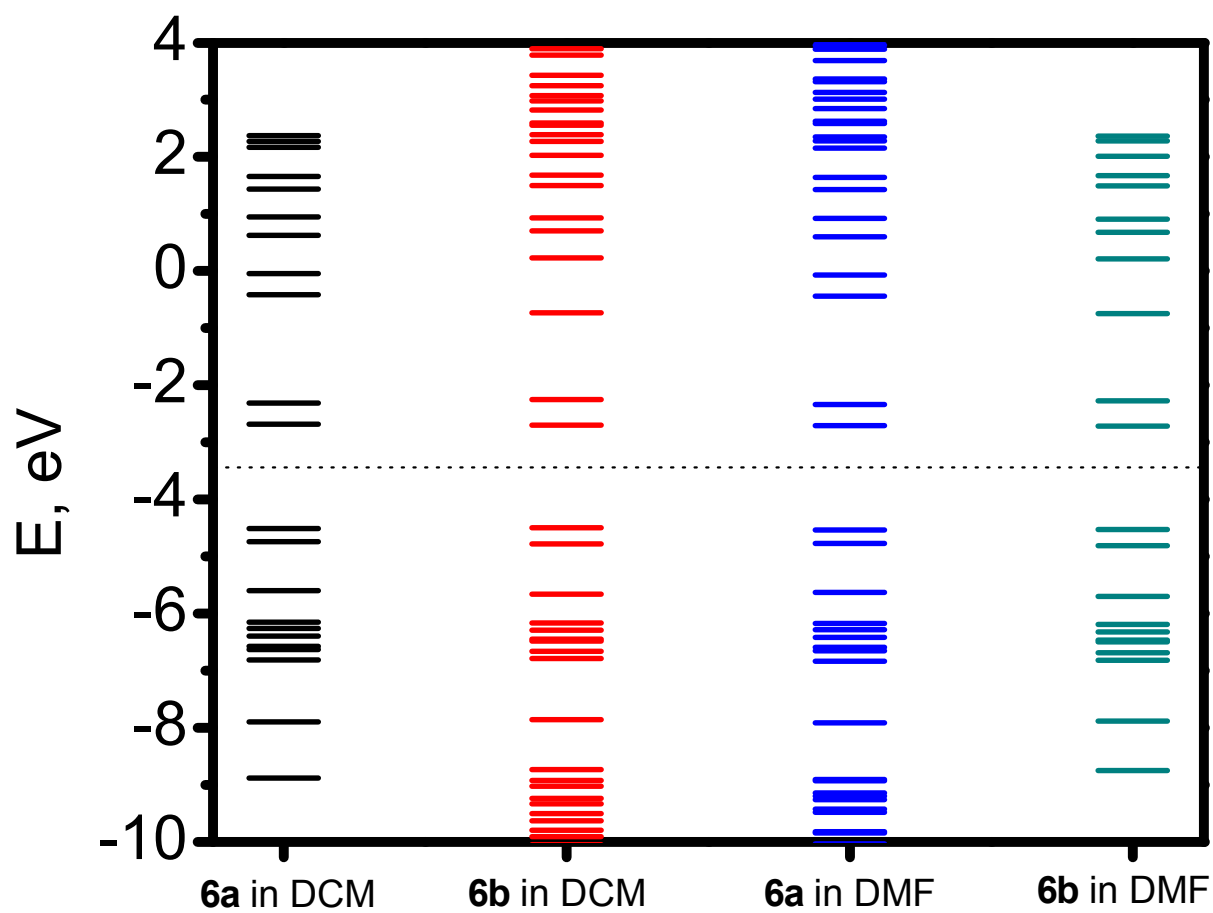
ESI Figure 1. Structure of corroles and parent corrole **6**.



ESI Figure 2. Experimental UV-vis spectrum of **5** (top) and PCM-TDDFT predicted UV-vis spectra of individual tautomers of parent corroles **6a** and **6b** in DCM.



ESI Figure 3. Experimental UV-vis spectrum of **5** (top) and PCM-TDDFT predicted UV-vis spectra of individual tautomers of parent corroles **6a** and **6b** in DMF.



ESI Figure 4. PCM-DFT predicted energies of individual tautomers of parent corroles **6a** and **6b** in DCM and DMF.

Corrole 6a in DCM

Coordinates:

C	-2.64384	2.92359	0.27198
C	-3.60258	1.91126	0.318
C	-2.96842	0.68304	-0.00667
C	-1.41009	2.33587	-0.08855
C	-0.02293	2.6684	-0.12798
C	2.08594	2.0966	-0.13503
C	2.04574	3.53819	-0.0513
C	0.71953	3.89599	-0.03667
C	-3.36313	-0.67117	0.00985
C	-2.46731	-1.73527	-0.00946
C	-2.71732	-3.12798	-0.18805
C	-1.5201	-3.80109	-0.16606
C	-0.46635	-2.85832	0.03132
C	0.90378	-3.09016	0.08678
C	1.95126	-2.15182	0.09689
C	3.35626	-2.40995	0.17873
C	4.02476	-1.20684	0.13021
C	3.05366	-0.16961	0.01595
C	3.182	1.2237	-0.05495
N	-1.67236	1.01367	-0.27522
H	-0.99104	0.40515	-0.70092
N	0.81307	1.61583	-0.20132
N	1.82888	-0.79592	0.00566
H	1.01298	-0.19263	-0.12907
N	-1.07568	-1.61237	0.09918
H	-0.6905	-0.8975	0.70488
H	4.18484	1.63796	-0.00776
H	1.20771	-4.13245	0.08977
H	-4.42126	-0.90799	0.04903
H	3.79064	-3.39723	0.27072
H	5.09523	-1.05165	0.17261
H	2.90392	4.19703	0.01327
H	0.3061	4.895	0.02946
H	-2.79644	3.96508	0.52263
H	-4.63869	2.01878	0.61194
H	-3.69839	-3.55202	-0.36075
H	-1.36772	-4.86267	-0.31386

Frequencies:

		1	2	3
Frequencies	--	68.6649	75.5566	92.9392

TDDFT data:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.0569	2.2524	550.47	18166.3		
=	=	=	=	=	=	77->79	-0.20942
=	=	=	=	=	=	77->80	0.31593
=	=	=	=	=	=	78->79	0.56338
=	=	=	=	=	=	78->80	0.18418
2	Singlet-A	0.0298	2.3523	527.07	18972.8		
=	=	=	=	=	=	77->79	0.48211
=	=	=	=	=	=	77->80	0.13526
=	=	=	=	=	=	78->79	0.24323
=	=	=	=	=	=	78->80	-0.42792
3	Singlet-A	0.1526	2.9885	414.88	24103.4		
=	=	=	=	=	=	76->79	0.59056
=	=	=	=	=	=	77->79	0.2307
=	=	=	=	=	=	77->80	0.1617
=	=	=	=	=	=	78->80	0.24248
4	Singlet-A	0.6826	3.1403	394.82	25328		
=	=	=	=	=	=	76->80	0.14678
=	=	=	=	=	=	77->79	-0.21266
=	=	=	=	=	=	77->80	0.51406
=	=	=	=	=	=	78->79	-0.29186
=	=	=	=	=	=	78->80	-0.24199
5	Singlet-A	0.8576	3.3021	375.48	26632.6		
=	=	=	=	=	=	76->79	-0.35113
=	=	=	=	=	=	76->80	0.13107
=	=	=	=	=	=	77->79	0.34821
=	=	=	=	=	=	77->80	0.22089
=	=	=	=	=	=	78->79	-0.15058
=	=	=	=	=	=	78->80	0.39459
6	Singlet-A	0.083	3.4369	360.74	27720.8		
=	=	=	=	=	=	74->79	-0.10327
=	=	=	=	=	=	75->79	-0.18199
=	=	=	=	=	=	76->79	0.11822
=	=	=	=	=	=	76->80	0.64387
=	=	=	=	=	=	77->80	-0.11101

	7	Singlet-A	0.0713	3.5706	347.24	28798.5		
=	=	=	=	=	=	=	73->79	0.22186
=	=	=	=	=	=	=	75->79	0.62935
=	=	=	=	=	=	=	76->80	0.15392
	8	Singlet-A	0.0432	3.7279	332.59	30067		
=	=	=	=	=	=	=	73->79	0.1109
=	=	=	=	=	=	=	74->79	0.66401
=	=	=	=	=	=	=	75->79	-0.15392
	9	Singlet-A	0.0335	3.8265	324.01	30863.2		
=	=	=	=	=	=	=	73->79	0.63085
=	=	=	=	=	=	=	74->79	-0.13232
=	=	=	=	=	=	=	75->79	-0.16831
=	=	=	=	=	=	=	75->80	-0.2032
	10	Singlet-A	0.0328	3.9261	315.79	31666.6		
=	=	=	=	=	=	=	73->79	0.17489
=	=	=	=	=	=	=	74->80	0.14619
=	=	=	=	=	=	=	75->80	0.64216
=	=	=	=	=	=	=	78->81	0.10779
	11	Singlet-A	0.0169	4.041	306.81	32593.5		
=	=	=	=	=	=	=	71->79	-0.16484
=	=	=	=	=	=	=	72->79	0.64805
=	=	=	=	=	=	=	74->80	-0.11089
	12	Singlet-A	0.0333	4.1255	300.53	33274.5		
=	=	=	=	=	=	=	71->79	0.43439
=	=	=	=	=	=	=	73->80	-0.26976
=	=	=	=	=	=	=	74->80	0.33085
=	=	=	=	=	=	=	77->81	0.13494
=	=	=	=	=	=	=	78->81	0.26256
	13	Singlet-A	0.0205	4.131	300.13	33318.9		
=	=	=	=	=	=	=	72->79	0.13472
=	=	=	=	=	=	=	73->80	0.45415
=	=	=	=	=	=	=	74->80	0.45792
=	=	=	=	=	=	=	75->80	-0.1336
=	=	=	=	=	=	=	78->81	-0.16887
	14	Singlet-A	0.0109	4.2022	295.05	33892.6		
=	=	=	=	=	=	=	71->79	0.32074
=	=	=	=	=	=	=	73->80	0.43038
=	=	=	=	=	=	=	74->80	-0.33162
=	=	=	=	=	=	=	78->81	0.21504
=	=	=	=	=	=	=	78->82	-0.10927
	15	Singlet-A	0.0791	4.3067	287.89	34735.5		
=	=	=	=	=	=	=	70->79	0.29857
=	=	=	=	=	=	=	71->79	-0.26486

=	=	=	=	=	=	71->80	-0.11545
=	=	=	=	=	=	77->81	-0.19132
=	=	=	=	=	=	78->81	0.43323
=	=	=	=	=	=	78->82	0.21321
	16	Singlet-A	0.0116	4.3516	284.92	35097.6	
=	=	=	=	=	=	70->79	0.48929
=	=	=	=	=	=	71->80	0.41648
=	=	=	=	=	=	72->80	0.11498
=	=	=	=	=	=	78->81	-0.16216
	17	Singlet-A	0.057	4.4566	278.2	35945.4	
=	=	=	=	=	=	70->80	0.14239
=	=	=	=	=	=	71->80	-0.13904
=	=	=	=	=	=	72->80	0.64405
	18	Singlet-A	0.0152	4.5845	270.44	36976.8	
=	=	=	=	=	=	70->80	0.39751
=	=	=	=	=	=	71->79	-0.20113
=	=	=	=	=	=	71->80	0.23185
=	=	=	=	=	=	72->80	-0.12968
=	=	=	=	=	=	77->81	0.42041
=	=	=	=	=	=	78->81	0.14216
	19	Singlet-A	0.1737	4.6554	266.32	37548.8	
=	=	=	=	=	=	70->79	-0.1358
=	=	=	=	=	=	70->80	-0.34427
=	=	=	=	=	=	77->81	0.26385
=	=	=	=	=	=	77->82	-0.14431
=	=	=	=	=	=	78->82	0.48268
	20	Singlet-A	0.1505	4.7366	261.76	38202.9	
=	=	=	=	=	=	70->79	0.1374
=	=	=	=	=	=	70->80	0.12542
=	=	=	=	=	=	71->80	-0.32952
=	=	=	=	=	=	77->81	0.22579
=	=	=	=	=	=	77->82	0.44613
=	=	=	=	=	=	78->81	-0.20857
=	=	=	=	=	=	78->82	0.17857
	21	Singlet-A	0.0708	5.0964	243.28	41104.9	
=	=	=	=	=	=	70->79	-0.21215
=	=	=	=	=	=	71->80	0.20807
=	=	=	=	=	=	72->80	0.1069
=	=	=	=	=	=	77->81	-0.18349
=	=	=	=	=	=	77->82	0.31749
=	=	=	=	=	=	78->82	0.14614
=	=	=	=	=	=	78->83	0.43137
	22	Singlet-A	0.0159	5.2301	237.06	42183.4	

=	=	=	=	=	=	69->79	0.25335
=	=	=	=	=	=	70->80	0.30715
=	=	=	=	=	=	71->79	0.17526
=	=	=	=	=	=	72->79	0.11386
=	=	=	=	=	=	77->81	-0.22218
=	=	=	=	=	=	77->82	-0.25751
=	=	=	=	=	=	78->81	-0.12159
=	=	=	=	=	=	78->82	0.28311
=	=	=	=	=	=	78->84	0.16513
	23	Singlet-A	0.0139	5.3288	232.67	42979.3	
=	=	=	=	=	=	69->79	-0.17498
=	=	=	=	=	=	71->80	-0.1388
=	=	=	=	=	=	76->81	0.41039
=	=	=	=	=	=	76->82	-0.14464
=	=	=	=	=	=	77->82	-0.16543
=	=	=	=	=	=	78->83	0.41213
=	=	=	=	=	=	78->84	-0.13456
	24	Singlet-A	0.0376	5.4398	227.92	43875	
=	=	=	=	=	=	69->79	0.42738
=	=	=	=	=	=	76->81	0.26498
=	=	=	=	=	=	77->83	0.44708
	25	Singlet-A	0.0732	5.5172	224.72	44499.8	
=	=	=	=	=	=	69->79	-0.2025
=	=	=	=	=	=	69->80	0.10167
=	=	=	=	=	=	70->79	-0.1515
=	=	=	=	=	=	71->80	0.12605
=	=	=	=	=	=	76->81	0.37717
=	=	=	=	=	=	76->82	-0.22845
=	=	=	=	=	=	77->82	0.15977
=	=	=	=	=	=	77->83	-0.11634
=	=	=	=	=	=	78->83	-0.28957
=	=	=	=	=	=	78->84	0.12115
	26	Singlet-A	0.026	5.5824	222.1	45024.8	
=	=	=	=	=	=	69->79	0.13164
=	=	=	=	=	=	70->80	-0.15611
=	=	=	=	=	=	77->81	0.10348
=	=	=	=	=	=	77->83	-0.18365
=	=	=	=	=	=	78->82	-0.13972
=	=	=	=	=	=	78->83	0.13292
=	=	=	=	=	=	78->84	0.57683
	27	Singlet-A	0.0418	5.6732	218.54	45758.2	
=	=	=	=	=	=	69->79	0.16828
=	=	=	=	=	=	76->81	0.21865

=	=	=	=	=	=	76->82	0.42822
=	=	=	=	=	=	77->83	-0.32127
=	=	=	=	=	=	77->84	0.25854
=	=	=	=	=	=	78->84	-0.1482
	28	Singlet-A	0.0281	5.7006	217.5	45977	
=	=	=	=	=	=	69->79	-0.24204
=	=	=	=	=	=	69->80	-0.1874
=	=	=	=	=	=	70->80	0.11949
=	=	=	=	=	=	76->81	0.12715
=	=	=	=	=	=	76->82	0.44181
=	=	=	=	=	=	77->83	0.27529
=	=	=	=	=	=	77->84	-0.12162
=	=	=	=	=	=	78->84	0.18776
	29	Singlet-A	0.0154	5.8509	211.91	47189.8	
=	=	=	=	=	=	69->79	-0.10906
=	=	=	=	=	=	69->80	0.53936
=	=	=	=	=	=	71->81	-0.10847
=	=	=	=	=	=	74->81	0.13542
=	=	=	=	=	=	77->83	0.12877
=	=	=	=	=	=	77->84	0.18091
=	=	=	=	=	=	78->84	0.11736
=	=	=	=	=	=	78->85	-0.12942
=	=	=	=	=	=	78->86	0.16039
	30	Singlet-A	0.0249	5.8762	210.99	47395.6	
=	=	=	=	=	=	69->80	-0.11423
=	=	=	=	=	=	73->81	0.30988
=	=	=	=	=	=	75->81	0.58724
	31	Singlet-A	0.0043	5.9275	209.17	47808	
=	=	=	=	=	=	69->80	-0.16044
=	=	=	=	=	=	74->81	0.49974
=	=	=	=	=	=	77->84	0.32635
=	=	=	=	=	=	78->85	0.27596
	32	Singlet-A	0.0026	5.9495	208.39	47986.9	
=	=	=	=	=	=	74->81	-0.39284
=	=	=	=	=	=	75->82	0.13034
=	=	=	=	=	=	77->84	0.21958
=	=	=	=	=	=	78->85	0.46349
	33	Singlet-A	0.0056	6.0225	205.87	48574.3	
=	=	=	=	=	=	69->80	0.15741
=	=	=	=	=	=	73->81	0.17324
=	=	=	=	=	=	74->81	0.13075
=	=	=	=	=	=	77->84	-0.37098
=	=	=	=	=	=	78->85	0.39958

=	=	=	=	=	=	78->86	0.22039
	34	Singlet-A	0.003	6.1777	200.7	49825.6	
=	=	=	=	=	=	72->81	-0.12256
=	=	=	=	=	=	73->81	0.32236
=	=	=	=	=	=	75->82	0.47158
=	=	=	=	=	=	77->85	-0.33045
	35	Singlet-A	0.0038	6.215	199.49	50127.8	
=	=	=	=	=	=	73->81	0.13264
=	=	=	=	=	=	75->82	0.28007
=	=	=	=	=	=	77->85	0.5978
=	=	=	=	=	=	77->86	0.11421
	36	Singlet-A	0.0001	6.2471	198.47	50385.4	
=	=	=	=	=	=	67->79	0.3152
=	=	=	=	=	=	68->79	0.62635
	37	Singlet-A	0.0095	6.2548	198.22	50449	
=	=	=	=	=	=	67->79	0.35224
=	=	=	=	=	=	68->79	-0.20764
=	=	=	=	=	=	72->81	-0.3195
=	=	=	=	=	=	73->81	0.17324
=	=	=	=	=	=	73->82	-0.20799
=	=	=	=	=	=	74->82	-0.14041
=	=	=	=	=	=	75->81	-0.12048
=	=	=	=	=	=	75->82	-0.21633
=	=	=	=	=	=	78->86	-0.19716
	38	Singlet-A	0.0083	6.2636	197.94	50520.4	
=	=	=	=	=	=	67->79	0.48726
=	=	=	=	=	=	68->79	-0.2284
=	=	=	=	=	=	73->81	-0.16435
=	=	=	=	=	=	73->82	0.20228
=	=	=	=	=	=	74->82	0.17642
=	=	=	=	=	=	75->81	0.10595
=	=	=	=	=	=	75->82	0.16211
=	=	=	=	=	=	76->83	-0.20997
	39	Singlet-A	0.0214	6.2977	196.87	50794.9	
=	=	=	=	=	=	67->79	0.10474
=	=	=	=	=	=	71->81	-0.31275
=	=	=	=	=	=	72->81	0.49588
=	=	=	=	=	=	72->82	0.1361
=	=	=	=	=	=	73->81	0.17448
=	=	=	=	=	=	73->82	-0.12179
=	=	=	=	=	=	78->86	-0.13719
	40	Singlet-A	0.0275	6.3074	196.57	50872.5	
=	=	=	=	=	=	67->79	0.1486

=	=	=	=	=	=	69->80	-0.10107
=	=	=	=	=	=	70->82	-0.11798
=	=	=	=	=	=	71->81	0.23267
=	=	=	=	=	=	72->81	0.14209
=	=	=	=	=	=	74->82	-0.20085
=	=	=	=	=	=	76->83	0.22739
=	=	=	=	=	=	76->84	-0.11462
=	=	=	=	=	=	78->86	0.4783

Corrole 6a in DMF

Coordinates:

C	-2.64331	2.92562	0.26921
C	-3.60229	1.91335	0.31598
C	-2.96769	0.6843	-0.00535
C	-1.40903	2.33684	-0.08849
C	-0.02161	2.66921	-0.12805
C	2.08754	2.09617	-0.13457
C	2.04797	3.53766	-0.05118
C	0.72143	3.89626	-0.03717
C	-3.36348	-0.66969	0.01121
C	-2.46834	-1.73444	-0.00833
C	-2.71907	-3.12683	-0.18932
C	-1.52208	-3.80053	-0.16814
C	-0.46806	-2.8584	0.03143
C	0.90213	-3.0911	0.08676
C	1.94994	-2.15312	0.09717
C	3.35516	-2.41197	0.17764
C	4.02428	-1.20918	0.12912
C	3.05359	-0.17105	0.01595
C	3.18331	1.22208	-0.05476
N	-1.67117	1.01427	-0.27265
H	-0.98883	0.40379	-0.69381
N	0.81426	1.61598	-0.20089
N	1.82818	-0.79694	0.00637
H	1.01193	-0.19384	-0.12605
N	-1.07648	-1.61205	0.10111
H	-0.69246	-0.90088	0.71197
H	4.18658	1.63534	-0.00792
H	1.20555	-4.13353	0.08888
H	-4.4219	-0.90534	0.04963

H	3.78908	-3.39956	0.26859
H	5.09487	-1.05448	0.17058
H	2.90649	4.19608	0.01352
H	0.3084	4.89548	0.02888
H	-2.79622	3.96783	0.51673
H	-4.63904	2.02147	0.60742
H	-3.7002	-3.55033	-0.36301
H	-1.3701	-4.86193	-0.31763

Frequencies:

		1	2	3
Frequencies	--	68.0869	75.3753	92.9302

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.059	2.2522	550.49	18165.6		
=	=	=	=	=	=	77->79	-0.20233
=	=	=	=	=	=	77->80	0.31702
=	=	=	=	=	=	78->79	0.5676
=	=	=	=	=	=	78->80	0.17757
2	Singlet-A	0.0295	2.3537	526.77	18983.6		
=	=	=	=	=	=	77->79	0.48619
=	=	=	=	=	=	77->80	0.13019
=	=	=	=	=	=	78->79	0.23502
=	=	=	=	=	=	78->80	-0.42954
3	Singlet-A	0.161	2.9948	414	24154.6		
=	=	=	=	=	=	76->79	0.58704
=	=	=	=	=	=	77->79	0.23404
=	=	=	=	=	=	77->80	0.16325
=	=	=	=	=	=	78->80	0.2471
4	Singlet-A	0.6905	3.1435	394.41	25354.3		
=	=	=	=	=	=	76->80	0.14149
=	=	=	=	=	=	77->79	-0.211
=	=	=	=	=	=	77->80	0.51659
=	=	=	=	=	=	78->79	-0.29226
=	=	=	=	=	=	78->80	-0.24071
5	Singlet-A	0.855	3.3041	375.24	26649.6		
=	=	=	=	=	=	76->79	-0.3593

=	=	=	=	=	=	76->80	0.12147
=	=	=	=	=	=	77->79	0.34566
=	=	=	=	=	=	77->80	0.21909
=	=	=	=	=	=	78->79	-0.14914
=	=	=	=	=	=	78->80	0.39392
	6	Singlet-A	0.074	3.4458	359.81	27792.4	
=	=	=	=	=	=	74->79	-0.10653
=	=	=	=	=	=	75->79	-0.18768
=	=	=	=	=	=	76->79	0.11161
=	=	=	=	=	=	76->80	0.64499
=	=	=	=	=	=	77->80	-0.10292
	7	Singlet-A	0.0719	3.5733	346.98	28820.1	
=	=	=	=	=	=	73->79	0.22456
=	=	=	=	=	=	75->79	0.62666
=	=	=	=	=	=	76->80	0.16136
	8	Singlet-A	0.0429	3.7289	332.49	30076.1	
=	=	=	=	=	=	73->79	0.12569
=	=	=	=	=	=	74->79	0.66051
=	=	=	=	=	=	75->79	-0.15789
	9	Singlet-A	0.0345	3.8232	324.29	30836.6	
=	=	=	=	=	=	73->79	0.63052
=	=	=	=	=	=	74->79	-0.14776
=	=	=	=	=	=	75->79	-0.16804
=	=	=	=	=	=	75->80	-0.19233
	10	Singlet-A	0.0316	3.9313	315.38	31707.8	
=	=	=	=	=	=	73->79	0.16345
=	=	=	=	=	=	74->80	0.1467
=	=	=	=	=	=	75->80	0.64226
=	=	=	=	=	=	78->81	0.11182
	11	Singlet-A	0.0196	4.0308	307.59	32510.8	
=	=	=	=	=	=	71->79	-0.12983
=	=	=	=	=	=	72->79	0.65963
=	=	=	=	=	=	74->80	-0.10654
	12	Singlet-A	0.0337	4.1243	300.62	33264.6	
=	=	=	=	=	=	71->79	0.44573
=	=	=	=	=	=	73->80	-0.30662
=	=	=	=	=	=	74->80	0.27049
=	=	=	=	=	=	77->81	0.13399
=	=	=	=	=	=	78->81	0.28534
	13	Singlet-A	0.017	4.1339	299.92	33342.2	
=	=	=	=	=	=	72->79	0.12548
=	=	=	=	=	=	73->80	0.42953
=	=	=	=	=	=	74->80	0.48763

=	=	=	=	=	=	75->80	-0.14211
=	=	=	=	=	=	78->81	-0.14542
14	Singlet-A	0.0108	4.2036	294.95	33904.1		
=	=	=	=	=	=	71->79	0.31156
=	=	=	=	=	=	73->80	0.43304
=	=	=	=	=	=	74->80	-0.34529
=	=	=	=	=	=	78->81	0.20648
=	=	=	=	=	=	78->82	0.10989
15	Singlet-A	0.0811	4.3042	288.05	34716.2		
=	=	=	=	=	=	70->79	0.28862
=	=	=	=	=	=	71->79	-0.2698
=	=	=	=	=	=	71->80	-0.12765
=	=	=	=	=	=	74->80	0.10156
=	=	=	=	=	=	77->81	-0.18795
=	=	=	=	=	=	78->81	0.43872
=	=	=	=	=	=	78->82	-0.20777
16	Singlet-A	0.0101	4.3537	284.78	35114.8		
=	=	=	=	=	=	70->79	0.49565
=	=	=	=	=	=	71->80	0.42294
=	=	=	=	=	=	78->81	-0.1571
17	Singlet-A	0.0575	4.452	278.49	35907.9		
=	=	=	=	=	=	70->80	0.13311
=	=	=	=	=	=	72->80	0.65909
18	Singlet-A	0.0145	4.5839	270.48	36971.3		
=	=	=	=	=	=	70->80	0.40463
=	=	=	=	=	=	71->79	-0.2024
=	=	=	=	=	=	71->80	0.21755
=	=	=	=	=	=	72->80	-0.1341
=	=	=	=	=	=	77->81	0.42258
=	=	=	=	=	=	78->81	0.14021
19	Singlet-A	0.1742	4.6548	266.36	37543.2		
=	=	=	=	=	=	70->79	0.13646
=	=	=	=	=	=	70->80	0.33951
=	=	=	=	=	=	77->81	-0.26741
=	=	=	=	=	=	77->82	-0.14191
=	=	=	=	=	=	78->82	0.48512
20	Singlet-A	0.1506	4.7373	261.72	38208.8		
=	=	=	=	=	=	70->79	-0.13869
=	=	=	=	=	=	70->80	-0.12265
=	=	=	=	=	=	71->80	0.33557
=	=	=	=	=	=	77->81	-0.22486
=	=	=	=	=	=	77->82	0.44544
=	=	=	=	=	=	78->81	0.20873

=	=	=	=	=	=	=	78->82	0.17615
	21	Singlet-A	0.0711	5.0985	243.18	41121.8		
=	=	=	=	=	=	=	70->79	-0.21054
=	=	=	=	=	=	=	71->80	0.21476
=	=	=	=	=	=	=	77->81	-0.18286
=	=	=	=	=	=	=	77->82	-0.31979
=	=	=	=	=	=	=	78->82	-0.14643
=	=	=	=	=	=	=	78->83	0.43159
	22	Singlet-A	0.0157	5.2321	236.97	42199.4		
=	=	=	=	=	=	=	69->79	0.25695
=	=	=	=	=	=	=	70->80	0.30477
=	=	=	=	=	=	=	71->79	0.18413
=	=	=	=	=	=	=	77->81	-0.2209
=	=	=	=	=	=	=	77->82	0.25801
=	=	=	=	=	=	=	78->81	-0.1201
=	=	=	=	=	=	=	78->82	-0.28315
=	=	=	=	=	=	=	78->84	0.16715
	23	Singlet-A	0.0144	5.3362	232.35	43038.5		
=	=	=	=	=	=	=	69->79	-0.18502
=	=	=	=	=	=	=	71->80	-0.14357
=	=	=	=	=	=	=	76->81	0.40372
=	=	=	=	=	=	=	76->82	0.14382
=	=	=	=	=	=	=	77->82	0.16757
=	=	=	=	=	=	=	78->83	0.41124
=	=	=	=	=	=	=	78->84	-0.13586
	24	Singlet-A	0.0344	5.4409	227.88	43882.7		
=	=	=	=	=	=	=	69->79	0.43058
=	=	=	=	=	=	=	70->80	-0.10138
=	=	=	=	=	=	=	76->81	0.26726
=	=	=	=	=	=	=	77->83	0.44534
	25	Singlet-A	0.0794	5.5247	224.42	44559.3		
=	=	=	=	=	=	=	69->79	-0.19764
=	=	=	=	=	=	=	69->80	0.10504
=	=	=	=	=	=	=	70->79	-0.15055
=	=	=	=	=	=	=	71->80	0.12977
=	=	=	=	=	=	=	76->81	0.38212
=	=	=	=	=	=	=	76->82	0.22506
=	=	=	=	=	=	=	77->82	-0.15718
=	=	=	=	=	=	=	78->83	-0.2946
=	=	=	=	=	=	=	78->84	0.10623
	26	Singlet-A	0.0233	5.5798	222.2	45004.5		
=	=	=	=	=	=	=	69->79	0.11871
=	=	=	=	=	=	=	70->80	-0.15359

=	=	=	=	=	=	77->81	0.10236
=	=	=	=	=	=	77->83	-0.17733
=	=	=	=	=	=	78->82	0.13825
=	=	=	=	=	=	78->83	0.12884
=	=	=	=	=	=	78->84	0.58364
27	Singlet-A	0.0396	5.6811	218.24	45821.1		
=	=	=	=	=	=	69->79	-0.18579
=	=	=	=	=	=	71->81	-0.10053
=	=	=	=	=	=	76->81	-0.20806
=	=	=	=	=	=	76->82	0.3909
=	=	=	=	=	=	77->83	0.34783
=	=	=	=	=	=	77->84	-0.26953
=	=	=	=	=	=	78->84	0.1484
28	Singlet-A	0.0277	5.7071	217.25	46029.9		
=	=	=	=	=	=	69->79	0.22389
=	=	=	=	=	=	69->80	0.18405
=	=	=	=	=	=	70->80	-0.11573
=	=	=	=	=	=	76->81	-0.14102
=	=	=	=	=	=	76->82	0.4759
=	=	=	=	=	=	77->83	-0.25221
=	=	=	=	=	=	78->84	-0.17666
29	Singlet-A	0.0149	5.8514	211.89	47194.3		
=	=	=	=	=	=	69->79	-0.1084
=	=	=	=	=	=	69->80	0.53748
=	=	=	=	=	=	71->81	-0.11019
=	=	=	=	=	=	74->81	0.13552
=	=	=	=	=	=	77->83	0.13376
=	=	=	=	=	=	77->84	0.18922
=	=	=	=	=	=	78->84	0.11585
=	=	=	=	=	=	78->85	-0.12497
=	=	=	=	=	=	78->86	0.15515
30	Singlet-A	0.0255	5.878	210.93	47409.1		
=	=	=	=	=	=	69->80	-0.11193
=	=	=	=	=	=	73->81	0.31166
=	=	=	=	=	=	75->81	0.58582
31	Singlet-A	0.0051	5.929	209.12	47819.4		
=	=	=	=	=	=	69->80	-0.18011
=	=	=	=	=	=	74->81	0.53379
=	=	=	=	=	=	77->84	0.31464
=	=	=	=	=	=	78->85	0.20442
32	Singlet-A	0.0022	5.9591	208.06	48063.1		
=	=	=	=	=	=	73->81	-0.10729
=	=	=	=	=	=	74->81	-0.34523

=	=	=	=	=	=	75->82	-0.13553
=	=	=	=	=	=	77->84	0.29236
=	=	=	=	=	=	78->85	0.44497
33	Singlet-A	0.0058	6.0313	205.57	48645.2		
=	=	=	=	=	=	69->80	0.15469
=	=	=	=	=	=	73->81	0.17473
=	=	=	=	=	=	74->81	0.11339
=	=	=	=	=	=	77->84	-0.32508
=	=	=	=	=	=	78->85	0.45782
=	=	=	=	=	=	78->86	0.22302
34	Singlet-A	0.0039	6.182	200.56	49860.4		
=	=	=	=	=	=	72->81	0.13193
=	=	=	=	=	=	73->81	-0.34829
=	=	=	=	=	=	75->81	0.1075
=	=	=	=	=	=	75->82	0.49282
=	=	=	=	=	=	77->85	0.24248
35	Singlet-A	0.0045	6.2319	198.95	50263.9		
=	=	=	=	=	=	75->82	-0.22233
=	=	=	=	=	=	77->85	0.62649
=	=	=	=	=	=	77->86	0.11209
36	Singlet-A	0	6.2427	198.61	50349.9		
=	=	=	=	=	=	67->79	0.3749
=	=	=	=	=	=	68->79	0.58473
37	Singlet-A	0.0072	6.2509	198.35	50415.9		
=	=	=	=	=	=	67->79	0.46246
=	=	=	=	=	=	68->79	-0.32015
=	=	=	=	=	=	72->81	-0.31667
=	=	=	=	=	=	73->82	0.11297
=	=	=	=	=	=	75->82	0.14223
=	=	=	=	=	=	78->86	-0.11539
38	Singlet-A	0.0113	6.2633	197.95	50517.8		
=	=	=	=	=	=	67->79	0.34086
=	=	=	=	=	=	68->79	-0.19437
=	=	=	=	=	=	72->81	0.27972
=	=	=	=	=	=	73->81	-0.16924
=	=	=	=	=	=	73->82	-0.24087
=	=	=	=	=	=	74->82	-0.18809
=	=	=	=	=	=	75->81	0.11995
=	=	=	=	=	=	75->82	-0.21254
=	=	=	=	=	=	76->83	-0.19304
=	=	=	=	=	=	78->86	0.12122
39	Singlet-A	0.02	6.2885	197.16	50720.2		
=	=	=	=	=	=	67->79	0.10063

=	=	=	=	=	=	71->81	-0.247
=	=	=	=	=	=	72->81	0.45053
=	=	=	=	=	=	72->82	-0.1302
=	=	=	=	=	=	73->81	0.22558
=	=	=	=	=	=	73->82	0.18674
=	=	=	=	=	=	74->82	0.14828
=	=	=	=	=	=	75->81	-0.13752
=	=	=	=	=	=	75->82	0.12092
=	=	=	=	=	=	78->86	-0.14612
40	Singlet-A	0.0293	6.3162	196.3	50942.4		
=	=	=	=	=	=	67->79	0.10529
=	=	=	=	=	=	70->82	0.11622
=	=	=	=	=	=	71->81	0.27326
=	=	=	=	=	=	72->81	0.10521
=	=	=	=	=	=	74->82	0.19764
=	=	=	=	=	=	76->83	0.2047
=	=	=	=	=	=	76->84	-0.10962
=	=	=	=	=	=	78->86	0.4916

Corrole 5a in DCM

Coordinates:

C	1.60776	-4.26525	0.29858
C	2.82437	-3.59102	0.36972
C	2.61407	-2.24879	-0.04337
C	0.63411	-3.34868	-0.15475
C	-0.78614	-3.26326	-0.20494
C	-2.64161	-2.11796	-0.18528
C	-3.00515	-3.50667	-0.01428
C	-1.83462	-4.22428	-0.0222
C	3.42533	-1.08387	-0.03006
C	2.85632	0.20148	-0.09227
C	3.47535	1.43237	-0.44488
C	2.52532	2.42418	-0.44529
C	1.26674	1.85813	-0.08698
C	0.02606	2.51404	-0.01517
C	-1.25059	1.90365	0.05398
C	-2.51565	2.55646	0.19488
C	-3.50679	1.6038	0.16302
C	-2.88892	0.32781	0.02794
C	-3.45131	-0.96545	-0.04868

N	1.29514	-2.18242	-0.38574
H	0.83777	-1.39288	-0.81436
N	-1.2916	-2.02039	-0.3253
N	-1.53281	0.56773	-0.02617
H	-0.9337	-0.24254	-0.21045
N	1.50117	0.5018	0.09001
H	0.93463	-0.04853	0.72302
H	-2.64722	3.62294	0.30995
H	-4.57184	1.77667	0.22987
H	-4.00623	-3.891	0.13386
H	-1.71474	-5.29389	0.09908
H	1.41822	-5.28709	0.59944
H	3.76103	-3.98823	0.73683
H	4.51269	1.53215	-0.73359
H	2.67142	3.45736	-0.72735
C	4.89054	-1.23051	0.05079
C	5.55402	-2.20939	-0.70668
C	5.6571	-0.41203	0.89583
C	6.934	-2.35992	-0.62504
H	4.9785	-2.84067	-1.37798
C	7.03776	-0.56035	0.97204
H	5.15766	0.32973	1.5128
C	7.68245	-1.535	0.21283
H	7.42785	-3.1187	-1.22612
H	7.61069	0.08009	1.63727
H	8.76079	-1.65247	0.27518
C	-4.9193	-1.11842	0.0644
C	-5.62934	-1.85188	-0.8977
C	-5.63243	-0.55475	1.13266
C	-7.00812	-2.01056	-0.7983
H	-5.09079	-2.28502	-1.73615
C	-7.01135	-0.71335	1.23083
H	-5.09376	-0.00844	1.90202
C	-7.70473	-1.4405	0.26532
H	-7.5404	-2.57642	-1.55825
H	-7.5443	-0.2749	2.07033
H	-8.78148	-1.56409	0.34278
C	0.06414	4.00177	-0.06033
C	0.77579	4.72616	0.90557
C	-0.59666	4.71111	-1.07283
C	0.82365	6.11671	0.86294
H	1.2865	4.18893	1.70046
C	-0.5514	6.10156	-1.11459

H	-1.13932	4.16218	-1.83782
C	0.15874	6.80929	-0.14667
H	1.37659	6.66006	1.62458
H	-1.06566	6.63292	-1.91101
H	0.1947	7.8948	-0.18009

Frequencies:

		1	2	3
Frequencies	--	20.9577	33.9247	38.9207

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.2262	1.9983	620.46	16117.1		
=	=	=	=	=	=	137->139	0.14659
=	=	=	=	=	=	137->140	-0.28301
=	=	=	=	=	=	138->139	0.61008
=	=	=	=	=	=	138->140	0.15467
2	Singlet-A	0.0511	2.175	570.05	17542.3		
=	=	=	=	=	=	137->139	0.43515
=	=	=	=	=	=	138->139	-0.19888
=	=	=	=	=	=	138->140	0.50735
3	Singlet-A	0.7392	2.7478	451.22	22162.1		
=	=	=	=	=	=	136->139	-0.25868
=	=	=	=	=	=	137->139	0.47563
=	=	=	=	=	=	137->140	-0.11339
=	=	=	=	=	=	138->140	-0.40068
4	Singlet-A	1.0177	2.8287	438.3	22815.4		
=	=	=	=	=	=	136->139	-0.21694
=	=	=	=	=	=	137->140	0.5921
=	=	=	=	=	=	138->139	0.26259
5	Singlet-A	0.3886	2.991	414.52	24124.3		
=	=	=	=	=	=	136->139	0.60239
=	=	=	=	=	=	136->140	-0.14285
=	=	=	=	=	=	137->139	0.19021
=	=	=	=	=	=	137->140	0.13584
=	=	=	=	=	=	138->140	-0.18682
6	Singlet-A	0.0734	3.2657	379.66	26339.4		
=	=	=	=	=	=	135->139	0.12807
=	=	=	=	=	=	136->139	0.11443

=	=	=	=	=	=	=	136->140	0.65747
	7	Singlet-A	0.0585	3.3325	372.04	26878.8		
=	=	=	=	=	=	=	135->139	0.40558
=	=	=	=	=	=	=	138->141	0.55077
	8	Singlet-A	0.0199	3.3796	366.86	27258.4		
=	=	=	=	=	=	=	134->139	-0.24035
=	=	=	=	=	=	=	135->139	0.22931
=	=	=	=	=	=	=	138->141	-0.17545
=	=	=	=	=	=	=	138->142	0.55744
	9	Singlet-A	0.0417	3.3888	365.86	27332.9		
=	=	=	=	=	=	=	130->139	0.13114
=	=	=	=	=	=	=	131->139	-0.10271
=	=	=	=	=	=	=	134->139	-0.20226
=	=	=	=	=	=	=	135->139	0.38015
=	=	=	=	=	=	=	138->141	-0.2436
=	=	=	=	=	=	=	138->142	-0.32962
=	=	=	=	=	=	=	138->143	0.17419
=	=	=	=	=	=	=	138->144	-0.20842
	10	Singlet-A	0.0028	3.4144	363.12	27539.1		
=	=	=	=	=	=	=	133->139	0.16113
=	=	=	=	=	=	=	138->142	0.10311
=	=	=	=	=	=	=	138->143	0.56852
=	=	=	=	=	=	=	138->144	0.12936
=	=	=	=	=	=	=	138->145	0.29502
	11	Singlet-A	0.0135	3.4224	362.28	27603		
=	=	=	=	=	=	=	133->139	-0.16194
=	=	=	=	=	=	=	134->139	-0.32038
=	=	=	=	=	=	=	138->143	0.13445
=	=	=	=	=	=	=	138->144	0.49654
=	=	=	=	=	=	=	138->145	-0.26397
	12	Singlet-A	0.0031	3.4358	360.86	27711.6		
=	=	=	=	=	=	=	130->139	0.10107
=	=	=	=	=	=	=	132->139	0.17833
=	=	=	=	=	=	=	134->139	0.43032
=	=	=	=	=	=	=	135->139	0.23733
=	=	=	=	=	=	=	138->141	-0.232
=	=	=	=	=	=	=	138->144	0.30207
=	=	=	=	=	=	=	138->145	-0.15436
	13	Singlet-A	0.0036	3.4587	358.47	27896.3		
=	=	=	=	=	=	=	128->139	0.13304
=	=	=	=	=	=	=	132->139	0.15065
=	=	=	=	=	=	=	133->139	0.56329
=	=	=	=	=	=	=	134->139	-0.16544

=	=	=	=	=	=	=	138->145	-0.2791
	14	Singlet-A	0.0172	3.478	356.48	28052.1		
=	=	=	=	=	=	=	131->139	0.43835
=	=	=	=	=	=	=	132->139	0.22339
=	=	=	=	=	=	=	133->139	-0.11358
=	=	=	=	=	=	=	138->142	0.10879
=	=	=	=	=	=	=	138->143	0.19025
=	=	=	=	=	=	=	138->144	-0.1836
=	=	=	=	=	=	=	138->145	-0.22868
=	=	=	=	=	=	=	138->146	-0.28867
	15	Singlet-A	0.0076	3.4934	354.91	28176.2		
=	=	=	=	=	=	=	128->139	-0.13703
=	=	=	=	=	=	=	130->139	0.19586
=	=	=	=	=	=	=	131->139	0.21422
=	=	=	=	=	=	=	133->139	-0.10452
=	=	=	=	=	=	=	135->140	0.15374
=	=	=	=	=	=	=	138->144	-0.12972
=	=	=	=	=	=	=	138->146	0.57115
	16	Singlet-A	0.026	3.503	353.93	28254.2		
=	=	=	=	=	=	=	128->139	0.11775
=	=	=	=	=	=	=	130->139	0.39062
=	=	=	=	=	=	=	132->139	0.38924
=	=	=	=	=	=	=	134->139	-0.11354
=	=	=	=	=	=	=	138->142	-0.12198
=	=	=	=	=	=	=	138->145	0.31375
	17	Singlet-A	0.0165	3.5259	351.64	28438.2		
=	=	=	=	=	=	=	127->139	-0.15743
=	=	=	=	=	=	=	130->139	0.10818
=	=	=	=	=	=	=	131->139	0.40405
=	=	=	=	=	=	=	132->139	-0.34183
=	=	=	=	=	=	=	133->139	0.23509
=	=	=	=	=	=	=	138->143	-0.13003
=	=	=	=	=	=	=	138->144	0.12146
=	=	=	=	=	=	=	138->145	0.19162
	18	Singlet-A	0.0066	3.5726	347.04	28815.1		
=	=	=	=	=	=	=	128->139	-0.11447
=	=	=	=	=	=	=	129->139	0.60464
=	=	=	=	=	=	=	130->139	-0.22089
=	=	=	=	=	=	=	132->139	0.13702
	19	Singlet-A	0.001	3.6452	340.13	29400.5		
=	=	=	=	=	=	=	128->139	0.31312
=	=	=	=	=	=	=	129->139	-0.13036
=	=	=	=	=	=	=	130->139	-0.27373

=	=	=	=	=	=	131->139	0.13927
=	=	=	=	=	=	134->139	-0.12293
=	=	=	=	=	=	135->140	0.36723
=	=	=	=	=	=	137->141	-0.21637
=	=	=	=	=	=	138->145	0.10904
=	=	=	=	=	=	138->147	-0.10611
20	Singlet-A	0.0157	3.6498	339.7	29437.7		
=	=	=	=	=	=	128->139	0.5374
=	=	=	=	=	=	129->139	0.19238
=	=	=	=	=	=	130->139	0.11015
=	=	=	=	=	=	132->139	-0.168
=	=	=	=	=	=	133->139	-0.10264
=	=	=	=	=	=	134->139	0.13029
=	=	=	=	=	=	135->140	-0.16524
21	Singlet-A	0.0644	3.6944	335.6	29797.4		
=	=	=	=	=	=	128->139	0.13147
=	=	=	=	=	=	135->140	0.14502
=	=	=	=	=	=	137->141	0.63874
22	Singlet-A	0.0621	3.7156	333.68	29968.8		
=	=	=	=	=	=	127->139	-0.18599
=	=	=	=	=	=	130->139	0.21367
=	=	=	=	=	=	131->139	-0.15438
=	=	=	=	=	=	135->140	0.42096
=	=	=	=	=	=	137->142	0.16942
=	=	=	=	=	=	137->143	0.1695
=	=	=	=	=	=	137->144	-0.15921
=	=	=	=	=	=	137->145	-0.19939
=	=	=	=	=	=	138->146	-0.14113
23	Singlet-A	0.0113	3.7307	332.33	30090.6		
=	=	=	=	=	=	137->142	0.64753
=	=	=	=	=	=	137->143	-0.19436
24	Singlet-A	0.0018	3.745	331.07	30205.1		
=	=	=	=	=	=	127->139	0.58033
=	=	=	=	=	=	132->139	-0.12167
=	=	=	=	=	=	133->140	0.20491
=	=	=	=	=	=	134->140	-0.15214
=	=	=	=	=	=	137->143	0.17115
25	Singlet-A	0.0202	3.7699	328.88	30406.2		
=	=	=	=	=	=	127->139	-0.10583
=	=	=	=	=	=	137->143	0.40004
=	=	=	=	=	=	137->144	0.52404
=	=	=	=	=	=	137->146	0.13393
26	Singlet-A	0.0164	3.7803	327.98	30489.7		

=	=	=	=	=	=	130->140	-0.22972
=	=	=	=	=	=	133->140	0.10282
=	=	=	=	=	=	134->140	0.34086
=	=	=	=	=	=	137->143	0.35223
=	=	=	=	=	=	137->144	-0.18182
=	=	=	=	=	=	137->145	0.33526
27	Singlet-A	0.0623	3.7968	326.55	30623.2		
=	=	=	=	=	=	127->139	0.20247
=	=	=	=	=	=	128->140	-0.11827
=	=	=	=	=	=	133->140	-0.31072
=	=	=	=	=	=	134->140	0.44726
=	=	=	=	=	=	137->144	0.13634
=	=	=	=	=	=	137->145	-0.26265
=	=	=	=	=	=	137->146	-0.10766
28	Singlet-A	0.0122	3.81	325.41	30730.5		
=	=	=	=	=	=	128->140	0.10021
=	=	=	=	=	=	132->140	-0.19015
=	=	=	=	=	=	133->140	0.48173
=	=	=	=	=	=	134->140	0.18543
=	=	=	=	=	=	137->143	-0.10879
=	=	=	=	=	=	137->144	0.22719
=	=	=	=	=	=	137->145	-0.21538
=	=	=	=	=	=	137->146	-0.19205
29	Singlet-A	0.0083	3.8208	324.5	30816.6		
=	=	=	=	=	=	128->140	0.17792
=	=	=	=	=	=	130->140	0.1051
=	=	=	=	=	=	131->140	-0.19816
=	=	=	=	=	=	132->140	0.57473
=	=	=	=	=	=	133->140	0.16242
=	=	=	=	=	=	137->144	0.13532
30	Singlet-A	0.0269	3.8262	324.04	30860.4		
=	=	=	=	=	=	130->140	0.21285
=	=	=	=	=	=	131->140	0.55674
=	=	=	=	=	=	132->140	0.13398
=	=	=	=	=	=	137->143	0.10115
=	=	=	=	=	=	137->144	-0.11869
=	=	=	=	=	=	137->146	-0.26718

Corrole 5a in DMF

Coordinates:

C	1.60764	-4.26642	0.29837
C	2.82436	-3.59228	0.36899
C	2.61362	-2.24928	-0.04204
C	0.63357	-3.3489	-0.15273
C	-0.78684	-3.26383	-0.20251
C	-2.6428	-2.11832	-0.18362
C	-3.00608	-3.5069	-0.01165
C	-1.83511	-4.2247	-0.01885
C	3.42522	-1.08457	-0.02941
C	2.85643	0.20099	-0.09212
C	3.47536	1.43105	-0.44766
C	2.52541	2.42306	-0.44839
C	1.26739	1.85762	-0.08722
C	0.02666	2.51397	-0.01518
C	-1.25003	1.90378	0.05383
C	-2.51535	2.55702	0.19272
C	-3.50674	1.60471	0.16069
C	-2.88921	0.32806	0.02737
C	-3.45237	-0.96491	-0.04841
N	1.29432	-2.18239	-0.38288
H	0.83652	-1.39124	-0.80812
N	-1.29273	-2.02085	-0.32369
N	-1.53277	0.56781	-0.02583
H	-0.93272	-0.24236	-0.20657
N	1.50151	0.50158	0.09166
H	0.93802	-0.04531	0.73049
H	-2.64744	3.6236	0.30618
H	-4.57165	1.77873	0.22704
H	-4.00699	-3.89196	0.13596
H	-1.71497	-5.29416	0.1036
H	1.41845	-5.28903	0.59686
H	3.76146	-3.99086	0.73349
H	4.51234	1.53096	-0.73761
H	2.672	3.45573	-0.73201
C	4.89056	-1.23133	0.05053
C	5.55349	-2.21157	-0.70591
C	5.65765	-0.41116	0.89364
C	6.93364	-2.36191	-0.62502
H	4.97793	-2.84431	-1.37578
C	7.03848	-0.55934	0.9691
H	5.15904	0.33195	1.50964
C	7.68266	-1.53543	0.21104
H	7.42706	-3.12178	-1.22502

H	7.61186	0.08244	1.63259
H	8.76102	-1.65274	0.27283
C	-4.92057	-1.1173	0.06377
C	-5.62977	-1.85476	-0.89615
C	-5.63502	-0.54924	1.12904
C	-7.00875	-2.01309	-0.79763
H	-5.09084	-2.29174	-1.73239
C	-7.01418	-0.70734	1.22629
H	-5.09782	0.00061	1.8969
C	-7.7066	-1.43854	0.26295
H	-7.54012	-2.58217	-1.55577
H	-7.54798	-0.26513	2.06323
H	-8.78341	-1.56174	0.33971
C	0.06539	4.0018	-0.05997
C	0.77904	4.72512	0.90545
C	-0.59639	4.7122	-1.07123
C	0.82773	6.11576	0.86355
H	1.29086	4.18738	1.69928
C	-0.55024	6.10275	-1.11228
H	-1.14068	4.16455	-1.83601
C	0.1618	6.80945	-0.14482
H	1.38232	6.65823	1.62459
H	-1.06529	6.63492	-1.90761
H	0.1985	7.89492	-0.17766

Frequencies:

		1	2	3
Frequencies	--	20.8044	33.8429	38.7193

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.2318	1.9959	621.2	16097.9		
=	=	=	=	=	=	137->139	0.14023
=	=	=	=	=	=	137->140	-0.28279
=	=	=	=	=	=	138->139	0.61329
=	=	=	=	=	=	138->140	0.14848
2	Singlet-A	0.049	2.1751	570.03	17542.9		
=	=	=	=	=	=	137->139	0.43618
=	=	=	=	=	=	138->139	-0.19085

=	=	=	=	=	=	138->140	0.51004
	3	Singlet-A	0.7423	2.7483	451.12	22167.1	
=	=	=	=	=	=	136->139	-0.25439
=	=	=	=	=	=	137->139	0.47883
=	=	=	=	=	=	137->140	-0.10969
=	=	=	=	=	=	138->140	-0.40162
	4	Singlet-A	1.0406	2.8287	438.3	22815.4	
=	=	=	=	=	=	136->139	-0.20219
=	=	=	=	=	=	137->140	0.59616
=	=	=	=	=	=	138->139	0.26409
	5	Singlet-A	0.3692	2.9972	413.66	24174.4	
=	=	=	=	=	=	136->139	0.6096
=	=	=	=	=	=	136->140	-0.13938
=	=	=	=	=	=	137->139	0.18472
=	=	=	=	=	=	137->140	0.12495
=	=	=	=	=	=	138->140	-0.18291
	6	Singlet-A	0.0702	3.2728	378.83	26397.1	
=	=	=	=	=	=	135->139	0.14157
=	=	=	=	=	=	136->139	0.11252
=	=	=	=	=	=	136->140	0.65508
	7	Singlet-A	0.0677	3.3377	371.47	26920.1	
=	=	=	=	=	=	135->139	0.45103
=	=	=	=	=	=	136->140	-0.10019
=	=	=	=	=	=	138->141	0.50687
	8	Singlet-A	0.0433	3.383	366.49	27285.9	
=	=	=	=	=	=	131->139	0.14609
=	=	=	=	=	=	134->139	0.39384
=	=	=	=	=	=	135->139	-0.32761
=	=	=	=	=	=	138->141	0.27987
=	=	=	=	=	=	138->142	-0.30036
	9	Singlet-A	0.0111	3.3975	364.92	27403.3	
=	=	=	=	=	=	130->139	-0.11424
=	=	=	=	=	=	132->139	0.12483
=	=	=	=	=	=	135->139	-0.1899
=	=	=	=	=	=	138->141	0.12361
=	=	=	=	=	=	138->142	0.55601
=	=	=	=	=	=	138->143	-0.23705
=	=	=	=	=	=	138->145	0.11223
	10	Singlet-A	0.0113	3.4142	363.15	27536.8	
=	=	=	=	=	=	133->139	0.23768
=	=	=	=	=	=	134->139	0.33923
=	=	=	=	=	=	138->141	-0.1789
=	=	=	=	=	=	138->142	0.10817

=	=	=	=	=	=	138->143	0.39488
=	=	=	=	=	=	138->145	0.29153
11	Singlet-A	0.0086	3.4267	361.82	27638.1		
=	=	=	=	=	=	132->139	-0.14505
=	=	=	=	=	=	134->139	-0.31482
=	=	=	=	=	=	135->139	-0.17528
=	=	=	=	=	=	135->140	-0.10956
=	=	=	=	=	=	138->141	0.17823
=	=	=	=	=	=	138->143	0.39867
=	=	=	=	=	=	138->144	0.31731
=	=	=	=	=	=	138->145	0.1177
12	Singlet-A	0.0012	3.4348	360.96	27703.9		
=	=	=	=	=	=	130->139	0.1483
=	=	=	=	=	=	132->139	0.1323
=	=	=	=	=	=	134->139	0.139
=	=	=	=	=	=	135->139	0.14517
=	=	=	=	=	=	138->141	-0.1775
=	=	=	=	=	=	138->144	0.55395
=	=	=	=	=	=	138->145	-0.21974
13	Singlet-A	0.0038	3.4524	359.13	27845.1		
=	=	=	=	=	=	128->139	0.12868
=	=	=	=	=	=	132->139	0.12351
=	=	=	=	=	=	133->139	0.57078
=	=	=	=	=	=	134->139	-0.19859
=	=	=	=	=	=	135->139	-0.11024
=	=	=	=	=	=	138->144	-0.10372
=	=	=	=	=	=	138->145	-0.21782
14	Singlet-A	0.0178	3.4806	356.21	28073.3		
=	=	=	=	=	=	130->139	0.14482
=	=	=	=	=	=	131->139	0.49873
=	=	=	=	=	=	132->139	0.19124
=	=	=	=	=	=	138->142	0.11442
=	=	=	=	=	=	138->143	0.20874
=	=	=	=	=	=	138->144	-0.1175
=	=	=	=	=	=	138->145	-0.20257
=	=	=	=	=	=	138->146	0.23418
15	Singlet-A	0.0178	3.4929	354.96	28172.2		
=	=	=	=	=	=	128->139	0.15208
=	=	=	=	=	=	131->139	-0.12269
=	=	=	=	=	=	132->139	0.24948
=	=	=	=	=	=	135->140	-0.15506
=	=	=	=	=	=	138->142	-0.10346
=	=	=	=	=	=	138->144	0.11193

=	=	=	=	=	=	138->145	0.24575
=	=	=	=	=	=	138->146	0.51465
16	Singlet-A	0.0117	3.4988	354.36	28219.9		
=	=	=	=	=	=	129->139	0.12048
=	=	=	=	=	=	130->139	0.39352
=	=	=	=	=	=	132->139	0.34741
=	=	=	=	=	=	138->145	0.24077
=	=	=	=	=	=	138->146	-0.3105
17	Singlet-A	0.0165	3.5258	351.65	28437.4		
=	=	=	=	=	=	127->139	0.15327
=	=	=	=	=	=	129->139	-0.13587
=	=	=	=	=	=	130->139	-0.18757
=	=	=	=	=	=	131->139	-0.32636
=	=	=	=	=	=	132->139	0.33685
=	=	=	=	=	=	133->139	-0.21392
=	=	=	=	=	=	138->143	0.17646
=	=	=	=	=	=	138->145	-0.2783
18	Singlet-A	0.0083	3.5582	348.44	28699.3		
=	=	=	=	=	=	129->139	0.56612
=	=	=	=	=	=	130->139	-0.29837
=	=	=	=	=	=	132->139	0.13765
=	=	=	=	=	=	138->142	-0.10357
19	Singlet-A	0.0028	3.6417	340.46	29372		
=	=	=	=	=	=	128->139	0.15152
=	=	=	=	=	=	129->139	-0.2207
=	=	=	=	=	=	130->139	-0.24827
=	=	=	=	=	=	131->139	0.17023
=	=	=	=	=	=	132->139	0.112
=	=	=	=	=	=	134->139	-0.15218
=	=	=	=	=	=	135->140	0.41462
=	=	=	=	=	=	137->141	-0.1329
=	=	=	=	=	=	138->145	0.14259
=	=	=	=	=	=	138->147	-0.11693
20	Singlet-A	0.0159	3.6512	339.57	29449		
=	=	=	=	=	=	128->139	0.61978
=	=	=	=	=	=	129->139	0.1309
=	=	=	=	=	=	132->139	-0.10477
=	=	=	=	=	=	133->139	-0.12933
=	=	=	=	=	=	137->141	-0.10472
21	Singlet-A	0.0437	3.7075	334.41	29903.4		
=	=	=	=	=	=	135->140	0.2001
=	=	=	=	=	=	137->141	0.62598
22	Singlet-A	0.0751	3.7159	333.66	29970.6		

=	=	=	=	=	=	127->139	-0.21871
=	=	=	=	=	=	128->139	-0.11711
=	=	=	=	=	=	130->139	0.18951
=	=	=	=	=	=	131->139	-0.1846
=	=	=	=	=	=	135->140	0.3806
=	=	=	=	=	=	137->141	-0.19897
=	=	=	=	=	=	137->142	0.13228
=	=	=	=	=	=	137->143	0.16967
=	=	=	=	=	=	137->145	-0.20684
=	=	=	=	=	=	138->146	0.14126
	23	Singlet-A	0.0008	3.7405	331.46	30169.6	
=	=	=	=	=	=	127->139	0.57023
=	=	=	=	=	=	129->139	0.10665
=	=	=	=	=	=	132->139	-0.1282
=	=	=	=	=	=	133->140	0.21352
=	=	=	=	=	=	134->140	-0.13875
=	=	=	=	=	=	135->140	0.11323
=	=	=	=	=	=	137->142	0.12317
=	=	=	=	=	=	137->143	0.10244
	24	Singlet-A	0.0158	3.7477	330.83	30227	
=	=	=	=	=	=	137->142	0.63669
=	=	=	=	=	=	137->143	-0.22824
	25	Singlet-A	0.0071	3.7788	328.11	30477.6	
=	=	=	=	=	=	130->140	-0.20171
=	=	=	=	=	=	133->140	0.10386
=	=	=	=	=	=	134->140	0.43999
=	=	=	=	=	=	137->143	0.24203
=	=	=	=	=	=	137->144	-0.27636
=	=	=	=	=	=	137->145	0.21264
=	=	=	=	=	=	137->146	0.11473
	26	Singlet-A	0.0358	3.7861	327.47	30537.1	
=	=	=	=	=	=	131->140	0.10516
=	=	=	=	=	=	137->143	0.38305
=	=	=	=	=	=	137->144	0.51789
=	=	=	=	=	=	137->146	-0.14448
	27	Singlet-A	0.0548	3.7943	326.77	30602.6	
=	=	=	=	=	=	127->139	0.18953
=	=	=	=	=	=	128->140	-0.14013
=	=	=	=	=	=	133->140	-0.35421
=	=	=	=	=	=	134->140	0.35865
=	=	=	=	=	=	137->143	-0.17532
=	=	=	=	=	=	137->144	0.12316
=	=	=	=	=	=	137->145	-0.2908

	28	Singlet-A	0.0164	3.8072	325.66	30706.9		
=	=	=	=	=	=	=	128->140	0.13348
=	=	=	=	=	=	=	133->140	0.47823
=	=	=	=	=	=	=	134->140	0.19724
=	=	=	=	=	=	=	137->143	-0.24826
=	=	=	=	=	=	=	137->144	0.25749
=	=	=	=	=	=	=	137->145	-0.12323
=	=	=	=	=	=	=	137->146	0.19092
	29	Singlet-A	0.0091	3.8116	325.28	30742.7		
=	=	=	=	=	=	=	131->140	-0.13677
=	=	=	=	=	=	=	132->140	0.63237
=	=	=	=	=	=	=	137->144	0.12347
=	=	=	=	=	=	=	137->145	0.12155
	30	Singlet-A	0.0156	3.8262	324.04	30860.4		
=	=	=	=	=	=	=	130->140	0.27295
=	=	=	=	=	=	=	131->140	0.54998
=	=	=	=	=	=	=	137->143	0.11699
=	=	=	=	=	=	=	137->144	-0.11916
=	=	=	=	=	=	=	137->145	0.11925
=	=	=	=	=	=	=	137->146	0.21714

Corrole 6b in DCM

Coordinates:

C	0.44724	-3.88113	-0.29949
C	-0.94833	-3.91347	-0.35288
C	-1.43983	-2.64004	0.01204
C	0.83696	-2.59361	0.10886
C	2.0274	-1.81953	0.1285
C	3.03495	0.20387	0.08671
C	4.04943	-0.79319	0.07651
C	3.4279	-2.03721	0.09725
C	-2.71779	-2.0461	0.00142
C	-2.93588	-0.67239	0.02849
C	-4.17319	0.04286	0.13502
C	-3.90709	1.38795	0.12314
C	-2.49086	1.56728	0.00516
C	-1.73927	2.73471	-0.05469
C	-0.33266	2.83705	-0.08949
C	0.3893	4.09452	-0.13134
C	1.71449	3.78522	-0.12432

C	1.80379	2.3413	-0.07103
C	2.99459	1.60643	-0.01158
N	-0.32693	-1.88476	0.30529
H	-0.37845	-1.10843	0.95153
N	1.85438	-0.47137	0.14465
N	0.53784	1.79809	-0.06231
N	-1.95312	0.30312	-0.02404
H	-1.01576	0.17169	-0.37745
H	-0.06668	5.07721	-0.16039
H	2.55863	4.46466	-0.14009
H	5.11505	-0.606	0.04666
H	3.91312	-3.00421	0.10306
H	1.11998	-4.67363	-0.5997
H	-1.55716	-4.74046	-0.69448
H	-5.14114	-0.43106	0.23684
H	-4.622	2.19648	0.20606
H	0.99571	0.08344	0.04516
H	-3.58844	-2.68984	-0.066
H	3.93275	2.15132	-0.05156
H	-2.29785	3.66619	-0.05464

Frequencies:

		1	2	3
Frequencies	--	68.3702	74.6811	92.19

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.0596	2.3006	538.92	18555.6		
=	=	=	=	=	=	77->79	0.30389
=	=	=	=	=	=	77->80	0.26116
=	=	=	=	=	=	78->79	0.50655
=	=	=	=	=	=	78->80	-0.28176
2	Singlet-A	0.055	2.3574	525.94	19013.6		
=	=	=	=	=	=	77->79	0.42698
=	=	=	=	=	=	77->80	-0.19038
=	=	=	=	=	=	78->79	-0.36906
=	=	=	=	=	=	78->80	-0.37451
3	Singlet-A	0.0098	3.1155	397.96	25128.2		

=	=	=	=	=	=	=	76->79	0.68503
	4	Singlet-A	0.7933	3.2021	387.19	25827.1		
=	=	=	=	=	=	=	76->80	-0.1741
=	=	=	=	=	=	=	77->79	0.39002
=	=	=	=	=	=	=	77->80	0.31102
=	=	=	=	=	=	=	78->79	-0.14834
=	=	=	=	=	=	=	78->80	0.4313
	5	Singlet-A	0.8729	3.2853	377.39	26497.8		
=	=	=	=	=	=	=	76->79	-0.14358
=	=	=	=	=	=	=	77->79	-0.23895
=	=	=	=	=	=	=	77->80	0.51058
=	=	=	=	=	=	=	78->79	-0.27254
=	=	=	=	=	=	=	78->80	-0.25607
	6	Singlet-A	0.0015	3.585	345.84	28915.1		
=	=	=	=	=	=	=	74->79	-0.31335
=	=	=	=	=	=	=	75->79	0.61154
=	=	=	=	=	=	=	76->80	-0.12881
	7	Singlet-A	0.1105	3.6319	341.37	29293.7		
=	=	=	=	=	=	=	75->79	0.11519
=	=	=	=	=	=	=	76->80	0.6504
=	=	=	=	=	=	=	78->81	-0.13546
	8	Singlet-A	0.0498	3.7106	334.13	29928.5		
=	=	=	=	=	=	=	74->79	0.60732
=	=	=	=	=	=	=	75->79	0.30623
	9	Singlet-A	0.0237	3.8718	320.22	31228.5		
=	=	=	=	=	=	=	71->79	-0.1082
=	=	=	=	=	=	=	72->79	0.12814
=	=	=	=	=	=	=	73->79	0.554
=	=	=	=	=	=	=	78->81	-0.36655
	10	Singlet-A	0.0268	3.9145	316.73	31572.6		
=	=	=	=	=	=	=	71->79	-0.14598
=	=	=	=	=	=	=	72->79	0.42782
=	=	=	=	=	=	=	73->79	-0.36468
=	=	=	=	=	=	=	74->79	-0.10096
=	=	=	=	=	=	=	75->80	-0.17928
=	=	=	=	=	=	=	78->81	-0.31327
	11	Singlet-A	0.0834	3.9587	313.19	31929.5		
=	=	=	=	=	=	=	71->79	0.16644
=	=	=	=	=	=	=	72->79	0.48538
=	=	=	=	=	=	=	73->79	0.18537
=	=	=	=	=	=	=	75->80	-0.106
=	=	=	=	=	=	=	78->81	0.37822
	12	Singlet-A	0.0136	4.0272	307.87	32481.2		

=	=	=	=	=	=	72->79	0.16936
=	=	=	=	=	=	73->80	0.11731
=	=	=	=	=	=	74->80	-0.33781
=	=	=	=	=	=	75->80	0.57144
13	Singlet-A	0.0157	4.1427	299.28	33413.5		
=	=	=	=	=	=	72->79	0.11456
=	=	=	=	=	=	74->80	0.59621
=	=	=	=	=	=	75->80	0.30573
=	=	=	=	=	=	77->81	-0.10091
14	Singlet-A	0.1459	4.1707	297.27	33639.5		
=	=	=	=	=	=	70->79	0.20813
=	=	=	=	=	=	71->79	0.47749
=	=	=	=	=	=	71->80	-0.11504
=	=	=	=	=	=	77->80	-0.11028
=	=	=	=	=	=	77->81	-0.38138
=	=	=	=	=	=	78->81	-0.14697
=	=	=	=	=	=	78->82	0.11459
15	Singlet-A	0.0256	4.3623	284.22	35184		
=	=	=	=	=	=	70->79	0.26562
=	=	=	=	=	=	70->80	0.25937
=	=	=	=	=	=	71->79	-0.23434
=	=	=	=	=	=	72->80	-0.20561
=	=	=	=	=	=	73->80	0.38546
=	=	=	=	=	=	77->81	-0.25965
=	=	=	=	=	=	78->81	0.12086
16	Singlet-A	0.0176	4.3648	284.06	35203.8		
=	=	=	=	=	=	72->80	0.60219
=	=	=	=	=	=	73->80	0.31684
17	Singlet-A	0.0651	4.4431	279.05	35835.9		
=	=	=	=	=	=	70->80	-0.22043
=	=	=	=	=	=	71->79	0.27401
=	=	=	=	=	=	72->80	-0.22738
=	=	=	=	=	=	73->80	0.41897
=	=	=	=	=	=	74->80	0.13118
=	=	=	=	=	=	77->81	0.29794
=	=	=	=	=	=	78->82	0.11454
18	Singlet-A	0.0211	4.4509	278.56	35898.9		
=	=	=	=	=	=	70->79	0.4932
=	=	=	=	=	=	71->80	0.34192
=	=	=	=	=	=	73->80	-0.18055
=	=	=	=	=	=	77->81	0.23359
=	=	=	=	=	=	78->82	0.12438
19	Singlet-A	0.0922	4.7943	258.61	38668.3		

=	=	=	=	=	=	70->80	0.43226
=	=	=	=	=	=	71->80	-0.20436
=	=	=	=	=	=	77->81	0.20098
=	=	=	=	=	=	78->82	0.43159
20	Singlet-A	0.0349	4.827	256.86	38931.7		
=	=	=	=	=	=	70->79	-0.20048
=	=	=	=	=	=	70->80	0.2086
=	=	=	=	=	=	71->80	0.44639
=	=	=	=	=	=	76->81	0.21184
=	=	=	=	=	=	77->81	-0.10196
=	=	=	=	=	=	77->82	0.30946
=	=	=	=	=	=	78->81	-0.1417
21	Singlet-A	0.0208	5.0395	246.03	40645.4		
=	=	=	=	=	=	70->80	-0.11277
=	=	=	=	=	=	76->81	0.63578
=	=	=	=	=	=	77->82	-0.22885
22	Singlet-A	0.1291	5.2076	238.09	42000.9		
=	=	=	=	=	=	69->79	-0.15542
=	=	=	=	=	=	70->79	-0.12868
=	=	=	=	=	=	70->80	-0.13482
=	=	=	=	=	=	71->79	-0.10405
=	=	=	=	=	=	71->80	0.1424
=	=	=	=	=	=	76->81	-0.123
=	=	=	=	=	=	77->81	-0.15565
=	=	=	=	=	=	77->82	-0.20493
=	=	=	=	=	=	78->82	0.35161
=	=	=	=	=	=	78->83	0.41527
23	Singlet-A	0.0638	5.3586	231.37	43220.8		
=	=	=	=	=	=	69->79	0.49396
=	=	=	=	=	=	78->82	-0.1045
=	=	=	=	=	=	78->83	0.3302
=	=	=	=	=	=	78->84	0.31672
24	Singlet-A	0.0075	5.4418	227.84	43890.4		
=	=	=	=	=	=	69->79	0.11115
=	=	=	=	=	=	70->80	-0.22947
=	=	=	=	=	=	71->79	-0.12657
=	=	=	=	=	=	72->81	0.12527
=	=	=	=	=	=	74->81	-0.11358
=	=	=	=	=	=	75->81	0.152
=	=	=	=	=	=	77->82	0.42859
=	=	=	=	=	=	77->83	0.23065
=	=	=	=	=	=	78->82	0.21718
25	Singlet-A	0.0432	5.5346	224.02	44638.9		

=	=	=	=	=	=	70->80	-0.10342
=	=	=	=	=	=	71->80	0.11483
=	=	=	=	=	=	74->81	-0.20924
=	=	=	=	=	=	77->81	-0.11409
=	=	=	=	=	=	77->83	-0.134
=	=	=	=	=	=	78->82	0.16867
=	=	=	=	=	=	78->83	-0.30542
=	=	=	=	=	=	78->84	0.47781
	26	Singlet-A	0.0345	5.5484	223.46	44750.7	
=	=	=	=	=	=	74->81	-0.43118
=	=	=	=	=	=	75->81	0.47168
=	=	=	=	=	=	77->82	-0.11449
=	=	=	=	=	=	78->82	-0.10029
=	=	=	=	=	=	78->84	-0.1419
	27	Singlet-A	0.0389	5.5792	222.23	44998.4	
=	=	=	=	=	=	69->79	0.35031
=	=	=	=	=	=	70->81	-0.12683
=	=	=	=	=	=	71->80	0.13999
=	=	=	=	=	=	74->81	0.13039
=	=	=	=	=	=	77->82	-0.21478
=	=	=	=	=	=	77->83	0.15542
=	=	=	=	=	=	78->82	0.13725
=	=	=	=	=	=	78->83	-0.2773
=	=	=	=	=	=	78->84	-0.27763
	28	Singlet-A	0.024	5.7069	217.25	46029.9	
=	=	=	=	=	=	69->79	-0.15273
=	=	=	=	=	=	69->80	0.21671
=	=	=	=	=	=	74->81	0.24479
=	=	=	=	=	=	75->81	0.237
=	=	=	=	=	=	77->83	0.448
=	=	=	=	=	=	77->84	0.20276
=	=	=	=	=	=	78->84	0.1655
	29	Singlet-A	0.0293	5.7597	215.26	46455.4	
=	=	=	=	=	=	69->80	0.34634
=	=	=	=	=	=	71->81	-0.10244
=	=	=	=	=	=	72->81	-0.10909
=	=	=	=	=	=	73->81	0.29917
=	=	=	=	=	=	74->81	-0.29354
=	=	=	=	=	=	75->81	-0.31743
=	=	=	=	=	=	77->83	0.1118
=	=	=	=	=	=	77->84	0.17225
	30	Singlet-A	0.0055	5.8466	212.06	47156.5	
=	=	=	=	=	=	69->80	-0.30238

=	=	=	=	=	=	71->81	0.13463
=	=	=	=	=	=	72->81	-0.23529
=	=	=	=	=	=	73->81	0.45961
=	=	=	=	=	=	77->83	0.10383
=	=	=	=	=	=	77->84	-0.22186
=	=	=	=	=	=	78->84	0.10228
31	Singlet-A	0.011	5.9014	210.09	47598.6		
=	=	=	=	=	=	69->80	0.33632
=	=	=	=	=	=	70->81	-0.10926
=	=	=	=	=	=	71->81	-0.1683
=	=	=	=	=	=	72->81	-0.1276
=	=	=	=	=	=	73->81	0.17481
=	=	=	=	=	=	74->81	0.23759
=	=	=	=	=	=	75->81	0.21459
=	=	=	=	=	=	77->83	-0.28056
=	=	=	=	=	=	77->84	-0.20214
32	Singlet-A	0.0001	5.9385	208.78	47897.3		
=	=	=	=	=	=	71->81	0.29706
=	=	=	=	=	=	73->81	0.18044
=	=	=	=	=	=	76->82	-0.28902
=	=	=	=	=	=	77->83	-0.20753
=	=	=	=	=	=	77->84	0.4367
33	Singlet-A	0.0178	6.0193	205.98	48548.4		
=	=	=	=	=	=	71->81	0.15624
=	=	=	=	=	=	72->81	0.21508
=	=	=	=	=	=	73->81	0.13595
=	=	=	=	=	=	76->82	0.55985
=	=	=	=	=	=	76->83	0.15585
=	=	=	=	=	=	77->84	0.12909
34	Singlet-A	0.0022	6.045	205.1	48756.7		
=	=	=	=	=	=	71->81	0.14721
=	=	=	=	=	=	78->85	0.66101
=	=	=	=	=	=	78->86	0.14008
35	Singlet-A	0.0002	6.067	204.36	48933.3		
=	=	=	=	=	=	68->79	0.70484
36	Singlet-A	0.1106	6.2027	199.89	50027.5		
=	=	=	=	=	=	70->81	-0.27854
=	=	=	=	=	=	71->81	-0.13857
=	=	=	=	=	=	72->81	0.4514
=	=	=	=	=	=	73->81	0.21015
=	=	=	=	=	=	75->82	-0.1275
=	=	=	=	=	=	76->82	-0.13674
=	=	=	=	=	=	77->85	-0.10903

=	=	=	=	=	=	78->86	0.14876
	37	Singlet-A	0.0093	6.2186	199.38	50155.5	
=	=	=	=	=	=	69->80	-0.11446
=	=	=	=	=	=	70->81	-0.17143
=	=	=	=	=	=	71->81	-0.29808
=	=	=	=	=	=	72->81	-0.21749
=	=	=	=	=	=	76->82	0.10382
=	=	=	=	=	=	77->84	0.20108
=	=	=	=	=	=	78->86	0.45985
	38	Singlet-A	0.0006	6.2577	198.13	50471.9	
=	=	=	=	=	=	67->79	0.70206
	39	Singlet-A	0.0134	6.3215	196.13	50986.6	
=	=	=	=	=	=	70->81	-0.30333
=	=	=	=	=	=	71->81	0.1262
=	=	=	=	=	=	77->85	0.55124
=	=	=	=	=	=	77->86	0.1438
	40	Singlet-A	0.0011	6.3551	195.09	51258.4	
=	=	=	=	=	=	66->79	0.67678
=	=	=	=	=	=	77->85	0.15661

Corrole 6b in DMF

Coordinates:

C	0.45226	-3.88009	-0.30133
C	-0.94329	-3.91414	-0.35443
C	-1.43633	-2.64196	0.01344
C	0.84027	-2.5928	0.11001
C	2.02972	-1.81728	0.12955
C	3.03483	0.20769	0.08709
C	4.05057	-0.78836	0.07322
C	3.43056	-2.03323	0.09416
C	-2.71502	-2.04975	0.00233
C	-2.93484	-0.67619	0.02962
C	-4.17364	0.03725	0.13225
C	-3.90957	1.38285	0.11966
C	-2.49315	1.56408	0.00492
C	-1.74318	2.73292	-0.05499
C	-0.3366	2.83722	-0.08881
C	0.38395	4.09541	-0.13207
C	1.70987	3.78764	-0.12493
C	1.80112	2.34393	-0.07006

C	2.99309	1.61024	-0.01152
N	-0.32444	-1.8855	0.30829
H	-0.37695	-1.11378	0.96002
N	1.85504	-0.46915	0.14803
N	0.53558	1.7991	-0.06022
N	-1.95344	0.30076	-0.02135
H	-1.01397	0.16966	-0.36904
H	-0.07325	5.07753	-0.16235
H	2.5532	4.4681	-0.14186
H	5.11587	-0.59971	0.04039
H	3.91665	-2.99982	0.09678
H	1.1261	-4.67103	-0.60319
H	-1.5513	-4.74107	-0.69764
H	-5.14111	-0.43819	0.23142
H	-4.62594	2.19042	0.19935
H	0.99516	0.08393	0.0512
H	-3.5848	-2.69447	-0.06692
H	3.93074	2.15591	-0.05328
H	-2.30327	3.66349	-0.05668

Frequencies:

		1	2	3
Frequencies	--	67.8703	74.4566	92.0582

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.0603	2.3005	538.95	18554.6		
=	=	=	=	=	=	77->79	0.29755
=	=	=	=	=	=	77->80	0.26444
=	=	=	=	=	=	78->79	0.51105
=	=	=	=	=	=	78->80	-0.27737
2	Singlet-A	0.0531	2.3584	525.72	19021.5		
=	=	=	=	=	=	77->79	0.43024
=	=	=	=	=	=	77->80	-0.18752
=	=	=	=	=	=	78->79	-0.36194
=	=	=	=	=	=	78->80	-0.37907
3	Singlet-A	0.0123	3.1286	396.3	25233.4		
=	=	=	=	=	=	76->79	0.6831

=	=	=	=	=	=	77->80	0.1106
	4	Singlet-A	0.8053	3.2027	387.12	25831.8	
=	=	=	=	=	=	76->80	-0.1699
=	=	=	=	=	=	77->79	0.39346
=	=	=	=	=	=	77->80	0.30714
=	=	=	=	=	=	78->79	-0.14705
=	=	=	=	=	=	78->80	0.43363
	5	Singlet-A	0.8736	3.2838	377.56	26485.9	
=	=	=	=	=	=	76->79	-0.15315
=	=	=	=	=	=	77->79	-0.23641
=	=	=	=	=	=	77->80	0.51065
=	=	=	=	=	=	78->79	-0.27375
=	=	=	=	=	=	78->80	-0.2522
	6	Singlet-A	0.0015	3.5896	345.4	28951.9	
=	=	=	=	=	=	74->79	-0.3067
=	=	=	=	=	=	75->79	0.61487
=	=	=	=	=	=	76->80	-0.1248
	7	Singlet-A	0.106	3.6383	340.77	29345.3	
=	=	=	=	=	=	75->79	0.11202
=	=	=	=	=	=	76->80	0.65197
=	=	=	=	=	=	78->81	-0.13726
	8	Singlet-A	0.0484	3.7153	333.71	29966.1	
=	=	=	=	=	=	74->79	0.60919
=	=	=	=	=	=	75->79	0.2999
	9	Singlet-A	0.0194	3.8692	320.44	31207.1	
=	=	=	=	=	=	72->79	0.1056
=	=	=	=	=	=	73->79	0.5856
=	=	=	=	=	=	78->81	-0.32812
	10	Singlet-A	0.0277	3.9103	317.07	31538.8	
=	=	=	=	=	=	71->79	-0.14249
=	=	=	=	=	=	72->79	0.46766
=	=	=	=	=	=	73->79	-0.30711
=	=	=	=	=	=	74->79	-0.10712
=	=	=	=	=	=	75->80	-0.18707
=	=	=	=	=	=	78->81	-0.31534
	11	Singlet-A	0.0891	3.9559	313.42	31906.1	
=	=	=	=	=	=	71->79	0.17777
=	=	=	=	=	=	72->79	0.4519
=	=	=	=	=	=	73->79	0.18957
=	=	=	=	=	=	78->81	0.40888
	12	Singlet-A	0.0147	4.0271	307.87	32481.2	
=	=	=	=	=	=	72->79	0.17077
=	=	=	=	=	=	73->80	0.12152

=	=	=	=	=	=	74->80	-0.324
=	=	=	=	=	=	75->80	0.57682
13	Singlet-A	0.0163	4.142	299.33	33407.9		
=	=	=	=	=	=	72->79	0.11113
=	=	=	=	=	=	74->80	0.60165
=	=	=	=	=	=	75->80	0.29574
14	Singlet-A	0.1425	4.1718	297.19	33648.5		
=	=	=	=	=	=	70->79	0.20729
=	=	=	=	=	=	71->79	0.47882
=	=	=	=	=	=	71->80	-0.11398
=	=	=	=	=	=	77->80	-0.10958
=	=	=	=	=	=	77->81	-0.38062
=	=	=	=	=	=	78->81	-0.14755
=	=	=	=	=	=	78->82	0.11412
15	Singlet-A	0.0101	4.3553	284.67	35128.4		
=	=	=	=	=	=	72->80	0.53792
=	=	=	=	=	=	73->80	0.4055
16	Singlet-A	0.0359	4.3605	284.33	35170.4		
=	=	=	=	=	=	70->79	0.25601
=	=	=	=	=	=	70->80	0.23233
=	=	=	=	=	=	71->79	-0.20679
=	=	=	=	=	=	72->80	-0.34169
=	=	=	=	=	=	73->80	0.34447
=	=	=	=	=	=	77->81	-0.24425
17	Singlet-A	0.062	4.4387	279.33	35799.9		
=	=	=	=	=	=	70->79	-0.13233
=	=	=	=	=	=	70->80	-0.23606
=	=	=	=	=	=	71->79	0.28513
=	=	=	=	=	=	72->80	-0.23349
=	=	=	=	=	=	73->80	0.39994
=	=	=	=	=	=	74->80	0.13798
=	=	=	=	=	=	77->81	0.28059
18	Singlet-A	0.0205	4.4512	278.54	35901.5		
=	=	=	=	=	=	70->79	0.48502
=	=	=	=	=	=	71->80	0.35621
=	=	=	=	=	=	73->80	-0.1074
=	=	=	=	=	=	77->81	0.26822
=	=	=	=	=	=	78->82	0.1363
19	Singlet-A	0.0943	4.7932	258.67	38659.3		
=	=	=	=	=	=	70->80	0.42923
=	=	=	=	=	=	71->80	-0.20856
=	=	=	=	=	=	77->81	0.20725
=	=	=	=	=	=	78->82	0.43248

	20	Singlet-A	0.0324	4.8283	256.79	38942.3		
=	=	=	=	=	=	=	70->79	-0.20518
=	=	=	=	=	=	=	70->80	0.21759
=	=	=	=	=	=	=	71->80	0.44352
=	=	=	=	=	=	=	76->81	0.20201
=	=	=	=	=	=	=	77->82	0.31147
=	=	=	=	=	=	=	78->81	-0.14461
	21	Singlet-A	0.0203	5.0522	245.41	40748.1		
=	=	=	=	=	=	=	70->80	-0.10608
=	=	=	=	=	=	=	76->81	0.63883
=	=	=	=	=	=	=	77->82	-0.2257
	22	Singlet-A	0.1314	5.2132	237.83	42046.8		
=	=	=	=	=	=	=	69->79	-0.1565
=	=	=	=	=	=	=	70->79	-0.12722
=	=	=	=	=	=	=	70->80	-0.13342
=	=	=	=	=	=	=	71->79	-0.10411
=	=	=	=	=	=	=	71->80	0.13765
=	=	=	=	=	=	=	76->81	-0.12628
=	=	=	=	=	=	=	77->81	-0.1535
=	=	=	=	=	=	=	77->82	-0.20246
=	=	=	=	=	=	=	78->82	0.35089
=	=	=	=	=	=	=	78->83	0.41913
	23	Singlet-A	0.0636	5.3604	231.3	43233.9		
=	=	=	=	=	=	=	69->79	0.49239
=	=	=	=	=	=	=	78->82	-0.10582
=	=	=	=	=	=	=	78->83	0.32375
=	=	=	=	=	=	=	78->84	0.32505
	24	Singlet-A	0.0071	5.4471	227.62	43932.9		
=	=	=	=	=	=	=	69->79	0.12343
=	=	=	=	=	=	=	70->80	-0.2288
=	=	=	=	=	=	=	71->79	-0.12522
=	=	=	=	=	=	=	72->81	0.12377
=	=	=	=	=	=	=	74->81	-0.11148
=	=	=	=	=	=	=	75->81	0.1537
=	=	=	=	=	=	=	77->82	0.42448
=	=	=	=	=	=	=	77->83	0.23419
=	=	=	=	=	=	=	78->82	0.21707
	25	Singlet-A	0.052	5.5299	224.21	44601		
=	=	=	=	=	=	=	70->80	-0.11563
=	=	=	=	=	=	=	71->80	0.10951
=	=	=	=	=	=	=	74->81	-0.14142
=	=	=	=	=	=	=	77->81	-0.12028
=	=	=	=	=	=	=	77->83	-0.13045

=	=	=	=	=	=	78->82	0.18564
=	=	=	=	=	=	78->83	-0.31492
=	=	=	=	=	=	78->84	0.49422
26	Singlet-A	0.0251	5.5552	223.19	44804.9		
=	=	=	=	=	=	74->81	-0.45535
=	=	=	=	=	=	75->81	0.47695
=	=	=	=	=	=	77->82	-0.12072
27	Singlet-A	0.04	5.5797	222.2	45004.5		
=	=	=	=	=	=	69->79	0.34729
=	=	=	=	=	=	70->81	-0.12533
=	=	=	=	=	=	71->80	0.1437
=	=	=	=	=	=	72->81	-0.10688
=	=	=	=	=	=	74->81	0.13302
=	=	=	=	=	=	77->82	-0.2233
=	=	=	=	=	=	77->83	0.15176
=	=	=	=	=	=	78->82	0.13893
=	=	=	=	=	=	78->83	-0.27888
=	=	=	=	=	=	78->84	-0.26983
28	Singlet-A	0.024	5.7085	217.19	46042.6		
=	=	=	=	=	=	69->79	-0.1547
=	=	=	=	=	=	69->80	0.21708
=	=	=	=	=	=	74->81	0.24787
=	=	=	=	=	=	75->81	0.23625
=	=	=	=	=	=	77->83	0.44812
=	=	=	=	=	=	77->84	0.2033
=	=	=	=	=	=	78->84	0.16127
29	Singlet-A	0.028	5.7621	215.17	46474.9		
=	=	=	=	=	=	69->80	0.35025
=	=	=	=	=	=	71->81	-0.10347
=	=	=	=	=	=	72->81	-0.11715
=	=	=	=	=	=	73->81	0.306
=	=	=	=	=	=	74->81	-0.28466
=	=	=	=	=	=	75->81	-0.31394
=	=	=	=	=	=	77->83	0.10109
=	=	=	=	=	=	77->84	0.176
30	Singlet-A	0.0053	5.8424	212.21	47123.1		
=	=	=	=	=	=	69->80	-0.30397
=	=	=	=	=	=	71->81	0.12919
=	=	=	=	=	=	72->81	-0.24828
=	=	=	=	=	=	73->81	0.4536
=	=	=	=	=	=	77->83	0.10101
=	=	=	=	=	=	77->84	-0.22006
=	=	=	=	=	=	78->84	0.1034

31	Singlet-A	0.0109	5.9026	210.05	47607.7		
=	=	=	=	=	=	69->80	0.33316
=	=	=	=	=	=	70->81	-0.11109
=	=	=	=	=	=	71->81	-0.16848
=	=	=	=	=	=	72->81	-0.12969
=	=	=	=	=	=	73->81	0.15893
=	=	=	=	=	=	74->81	0.24304
=	=	=	=	=	=	75->81	0.21898
=	=	=	=	=	=	77->82	0.10091
=	=	=	=	=	=	77->83	-0.28118
=	=	=	=	=	=	77->84	-0.20899
32	Singlet-A	0.0003	5.9367	208.84	47883.5		
=	=	=	=	=	=	71->81	0.30346
=	=	=	=	=	=	73->81	0.18363
=	=	=	=	=	=	74->81	0.1079
=	=	=	=	=	=	76->82	-0.24362
=	=	=	=	=	=	77->83	-0.21827
=	=	=	=	=	=	77->84	0.44586
33	Singlet-A	0.021	6.0322	205.54	48652.3		
=	=	=	=	=	=	71->81	0.13716
=	=	=	=	=	=	72->81	0.22634
=	=	=	=	=	=	73->81	0.13584
=	=	=	=	=	=	76->82	0.57305
=	=	=	=	=	=	76->83	0.15798
34	Singlet-A	0.0026	6.0609	204.56	48885.4		
=	=	=	=	=	=	71->81	0.15204
=	=	=	=	=	=	78->85	0.65827
=	=	=	=	=	=	78->86	0.14247
35	Singlet-A	0.0002	6.0673	204.35	48935.6		
=	=	=	=	=	=	68->79	0.70478
36	Singlet-A	0.1112	6.2027	199.89	50027.5		
=	=	=	=	=	=	70->81	-0.25049
=	=	=	=	=	=	71->81	-0.10894
=	=	=	=	=	=	72->81	0.46334
=	=	=	=	=	=	73->81	0.22702
=	=	=	=	=	=	75->82	-0.1194
=	=	=	=	=	=	76->82	-0.16731
=	=	=	=	=	=	77->85	-0.10264
37	Singlet-A	0.0061	6.225	199.17	50208.4		
=	=	=	=	=	=	69->80	-0.12165
=	=	=	=	=	=	70->81	-0.20441
=	=	=	=	=	=	71->81	-0.3157
=	=	=	=	=	=	72->81	-0.16021

=	=	=	=	=	=	77->84	0.19295
=	=	=	=	=	=	78->86	0.46425
	38	Singlet-A	0.0007	6.2539	198.25	50441.4	
=	=	=	=	=	=	67->79	0.70122
	39	Singlet-A	0.0216	6.3319	195.81	51069.9	
=	=	=	=	=	=	66->79	-0.16541
=	=	=	=	=	=	70->81	-0.36082
=	=	=	=	=	=	71->81	0.17988
=	=	=	=	=	=	77->85	0.45855
=	=	=	=	=	=	77->86	0.10933
	40	Singlet-A	0.0004	6.3544	195.11	51253.1	
=	=	=	=	=	=	66->79	0.67949
=	=	=	=	=	=	77->85	0.15139

Corrole 5b in DCM

Coordinates:

C	1.72543	-4.22039	0.25338
C	2.91587	-3.50035	0.3495
C	2.67299	-2.17574	-0.08027
C	0.73481	-3.35225	-0.23653
C	-0.68283	-3.34822	-0.27118
C	-2.63761	-2.22811	-0.18362
C	-2.9226	-3.61871	-0.09866
C	-1.71645	-4.30654	-0.15341
C	3.45126	-0.98929	-0.034
C	2.85588	0.28223	-0.08435
C	3.48484	1.5523	-0.26985
C	2.52173	2.52729	-0.27013
C	1.24425	1.90553	-0.10347
C	-0.02297	2.50046	-0.05063
C	-1.26366	1.80913	0.0114
C	-2.55398	2.46874	-0.02126
C	-3.4974	1.48982	-0.0071
C	-2.79104	0.22843	0.02777
C	-3.40272	-1.04567	-0.03076
N	1.35152	-2.14435	-0.45304
H	0.98626	-1.44016	-1.07923
N	-1.28675	-2.13057	-0.32669
N	-1.43203	0.46127	0.04185
N	1.49511	0.55407	-0.0154

H	0.79606	-0.06284	0.37517
H	-2.71588	3.53711	-0.06956
H	-4.57117	1.61179	-0.05751
H	-3.90654	-4.05281	0.01463
H	-1.57791	-5.37878	-0.11301
H	1.55853	-5.23704	0.58351
H	3.85053	-3.85726	0.7601
H	4.5462	1.69146	-0.42156
H	2.67635	3.58858	-0.40396
C	4.91563	-1.11378	0.11017
C	5.63104	-2.0328	-0.67367
C	5.62609	-0.34149	1.04245
C	7.00852	-2.16715	-0.53681
H	5.09851	-2.63141	-1.40762
C	7.00445	-0.47328	1.17464
H	5.08506	0.35022	1.6821
C	7.70197	-1.38597	0.38573
H	7.5432	-2.87925	-1.15972
H	7.5335	0.13096	1.90672
H	8.77824	-1.49034	0.49172
C	-4.87138	-1.17798	0.08236
C	-5.59342	-1.93773	-0.85067
C	-5.57515	-0.57166	1.13387
C	-6.97298	-2.07977	-0.73998
H	-5.06535	-2.40148	-1.67951
C	-6.95498	-0.71291	1.24277
H	-5.02691	-0.00235	1.87928
C	-7.65951	-1.4671	0.30652
H	-7.51422	-2.66491	-1.47871
H	-7.48009	-0.23952	2.06813
H	-8.73695	-1.57812	0.39287
C	-0.06075	3.99146	-0.09205
C	-0.49634	4.72536	1.01854
C	0.33461	4.68967	-1.23987
C	-0.53537	6.11666	0.98295
H	-0.80261	4.19531	1.91676
C	0.30021	6.08152	-1.27541
H	0.66215	4.13193	-2.1136
C	-0.13539	6.79957	-0.16394
H	-0.87451	6.66837	1.8558
H	0.60776	6.60491	-2.17693
H	-0.16448	7.88547	-0.19164
H	-0.87891	-1.19043	-0.22782

Frequencies:

		1	2	3
Frequencies	--	21.3463	32.1696	40.2217

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.3629	2.0513	604.42	16544.8		
=	=	=	=	=	=	137->139	0.10699
=	=	=	=	=	=	137->140	-0.24379
=	=	=	=	=	=	138->139	0.64166
=	=	=	=	=	=	138->140	0.12785
2	Singlet-A	0.0335	2.185	567.44	17623		
=	=	=	=	=	=	137->139	0.45768
=	=	=	=	=	=	138->139	-0.1575
=	=	=	=	=	=	138->140	0.5054
3	Singlet-A	0.8268	2.8663	432.56	23118.2		
=	=	=	=	=	=	135->139	-0.10599
=	=	=	=	=	=	137->139	0.48835
=	=	=	=	=	=	137->140	-0.11139
=	=	=	=	=	=	138->140	-0.43719
=	=	=	=	=	=	138->141	-0.12821
4	Singlet-A	0.5274	2.9709	417.32	23962.4		
=	=	=	=	=	=	136->139	0.47743
=	=	=	=	=	=	137->140	-0.46275
=	=	=	=	=	=	138->139	-0.17361
5	Singlet-A	0.6977	3.0203	410.51	24359.9		
=	=	=	=	=	=	136->139	0.50527
=	=	=	=	=	=	137->139	0.10353
=	=	=	=	=	=	137->140	0.4165
=	=	=	=	=	=	138->139	0.16089
6	Singlet-A	0.1018	3.247	381.84	26189		
=	=	=	=	=	=	134->139	-0.22059
=	=	=	=	=	=	135->139	0.60217
=	=	=	=	=	=	138->140	-0.10842
=	=	=	=	=	=	138->141	0.21932
7	Singlet-A	0.0414	3.3333	371.96	26884.6		
=	=	=	=	=	=	134->139	0.59638
=	=	=	=	=	=	138->141	0.30666
8	Singlet-A	0.0029	3.3897	365.77	27339.6		

=	=	=	=	=	=	130->139	0.15141
=	=	=	=	=	=	134->139	-0.10151
=	=	=	=	=	=	135->139	-0.11379
=	=	=	=	=	=	138->141	0.24776
=	=	=	=	=	=	138->142	0.61136
	9	Singlet-A	0.0009	3.4209	362.43	27591.5	
=	=	=	=	=	=	129->139	0.1405
=	=	=	=	=	=	133->139	-0.11053
=	=	=	=	=	=	134->139	-0.11427
=	=	=	=	=	=	135->139	-0.1446
=	=	=	=	=	=	138->141	0.28989
=	=	=	=	=	=	138->142	-0.21175
=	=	=	=	=	=	138->143	0.44915
=	=	=	=	=	=	138->144	-0.19335
=	=	=	=	=	=	138->145	0.1989
	10	Singlet-A	0.0161	3.4251	361.99	27625.1	
=	=	=	=	=	=	129->139	-0.10875
=	=	=	=	=	=	131->139	-0.2015
=	=	=	=	=	=	132->139	0.10237
=	=	=	=	=	=	133->139	0.10557
=	=	=	=	=	=	134->139	0.103
=	=	=	=	=	=	138->141	-0.15464
=	=	=	=	=	=	138->142	0.13532
=	=	=	=	=	=	138->143	0.34925
=	=	=	=	=	=	138->144	0.45382
=	=	=	=	=	=	138->145	0.16004
	11	Singlet-A	0.0017	3.4294	361.54	27659.5	
=	=	=	=	=	=	130->139	0.11791
=	=	=	=	=	=	131->139	0.16804
=	=	=	=	=	=	132->139	0.45976
=	=	=	=	=	=	133->139	0.34055
=	=	=	=	=	=	136->140	0.10191
=	=	=	=	=	=	138->141	0.21139
=	=	=	=	=	=	138->143	-0.15089
=	=	=	=	=	=	138->144	0.13295
	12	Singlet-A	0.0144	3.4406	360.36	27750	
=	=	=	=	=	=	131->139	-0.21531
=	=	=	=	=	=	136->140	-0.20871
=	=	=	=	=	=	138->143	-0.2642
=	=	=	=	=	=	138->145	0.55431
	13	Singlet-A	0.0065	3.4499	359.39	27824.9	
=	=	=	=	=	=	133->139	0.43199
=	=	=	=	=	=	134->139	0.14248

=	=	=	=	=	=	135->139	0.14994
=	=	=	=	=	=	136->140	0.11448
=	=	=	=	=	=	138->141	-0.16211
=	=	=	=	=	=	138->142	0.12825
=	=	=	=	=	=	138->143	0.17362
=	=	=	=	=	=	138->144	-0.38616
=	=	=	=	=	=	138->146	-0.11901
14	Singlet-A	0.0446	3.4711	357.19	27996.3		
=	=	=	=	=	=	131->139	-0.22253
=	=	=	=	=	=	133->139	-0.17033
=	=	=	=	=	=	136->140	0.53722
=	=	=	=	=	=	138->146	-0.29981
15	Singlet-A	0.0084	3.4986	354.38	28218.3		
=	=	=	=	=	=	129->139	-0.14755
=	=	=	=	=	=	131->139	0.52669
=	=	=	=	=	=	132->139	-0.13534
=	=	=	=	=	=	138->144	0.11693
=	=	=	=	=	=	138->145	0.2739
=	=	=	=	=	=	138->146	-0.23103
16	Singlet-A	0.0335	3.5122	353.01	28327.8		
=	=	=	=	=	=	129->139	0.16737
=	=	=	=	=	=	130->139	0.17223
=	=	=	=	=	=	132->139	-0.32966
=	=	=	=	=	=	133->139	0.13763
=	=	=	=	=	=	136->140	0.29339
=	=	=	=	=	=	138->145	0.13103
=	=	=	=	=	=	138->146	0.40738
17	Singlet-A	0.0072	3.5369	350.54	28527.4		
=	=	=	=	=	=	129->139	-0.10609
=	=	=	=	=	=	130->139	0.55683
=	=	=	=	=	=	131->139	0.12147
=	=	=	=	=	=	132->139	0.15183
=	=	=	=	=	=	133->139	-0.19379
=	=	=	=	=	=	138->141	-0.14171
=	=	=	=	=	=	138->143	0.10965
=	=	=	=	=	=	138->144	-0.14148
18	Singlet-A	0.0037	3.5488	349.37	28622.9		
=	=	=	=	=	=	128->139	-0.14678
=	=	=	=	=	=	129->139	0.22209
=	=	=	=	=	=	130->139	-0.26462
=	=	=	=	=	=	131->139	0.1255
=	=	=	=	=	=	132->139	0.29633
=	=	=	=	=	=	133->139	-0.21409

=	=	=	=	=	=	138->141	-0.17745
=	=	=	=	=	=	138->142	0.15373
=	=	=	=	=	=	138->145	0.112
=	=	=	=	=	=	138->146	0.27338
19	Singlet-A	0.0156	3.6273	341.81	29256		
=	=	=	=	=	=	128->139	-0.1093
=	=	=	=	=	=	129->139	0.4368
=	=	=	=	=	=	135->140	0.42069
=	=	=	=	=	=	137->141	-0.20117
=	=	=	=	=	=	138->146	-0.15791
20	Singlet-A	0.0213	3.6732	337.54	29626.1		
=	=	=	=	=	=	128->139	0.55306
=	=	=	=	=	=	129->139	-0.12465
=	=	=	=	=	=	132->139	0.12963
=	=	=	=	=	=	133->139	-0.1285
=	=	=	=	=	=	135->140	0.29466
=	=	=	=	=	=	138->147	-0.1162
21	Singlet-A	0.0236	3.7332	332.12	30109.6		
=	=	=	=	=	=	128->139	-0.22584
=	=	=	=	=	=	129->139	-0.21469
=	=	=	=	=	=	134->140	-0.25146
=	=	=	=	=	=	135->140	0.38278
=	=	=	=	=	=	137->141	0.28847
=	=	=	=	=	=	138->146	0.11224
=	=	=	=	=	=	138->147	0.17642
22	Singlet-A	0.045	3.7755	328.39	30451.6		
=	=	=	=	=	=	127->139	0.1096
=	=	=	=	=	=	128->139	-0.10867
=	=	=	=	=	=	134->140	0.52534
=	=	=	=	=	=	135->140	0.10777
=	=	=	=	=	=	137->141	0.30717
=	=	=	=	=	=	138->147	-0.23509
23	Singlet-A	0.0069	3.7958	326.63	30615.7		
=	=	=	=	=	=	127->139	0.52072
=	=	=	=	=	=	134->140	-0.22909
=	=	=	=	=	=	137->141	0.12783
=	=	=	=	=	=	137->142	0.33436
24	Singlet-A	0.0188	3.8024	326.07	30668.3		
=	=	=	=	=	=	127->139	-0.29324
=	=	=	=	=	=	128->139	0.15069
=	=	=	=	=	=	133->140	0.18292
=	=	=	=	=	=	137->141	0.21769
=	=	=	=	=	=	137->142	0.44657

=	=	=	=	=	=	=	138->147	0.25226
	25	Singlet-A	0.0187	3.8204	324.53	30813.8		
=	=	=	=	=	=	=	125->139	-0.11361
=	=	=	=	=	=	=	126->139	0.32475
=	=	=	=	=	=	=	127->139	0.21019
=	=	=	=	=	=	=	134->140	0.19221
=	=	=	=	=	=	=	137->142	-0.12787
=	=	=	=	=	=	=	137->143	0.18114
=	=	=	=	=	=	=	138->147	0.43138
	26	Singlet-A	0.0056	3.8403	322.85	30974.1		
=	=	=	=	=	=	=	126->139	0.10629
=	=	=	=	=	=	=	127->139	-0.10462
=	=	=	=	=	=	=	129->139	-0.14171
=	=	=	=	=	=	=	132->140	-0.11505
=	=	=	=	=	=	=	133->140	-0.15267
=	=	=	=	=	=	=	137->141	-0.28556
=	=	=	=	=	=	=	137->142	0.37112
=	=	=	=	=	=	=	137->143	0.14849
=	=	=	=	=	=	=	137->144	-0.18064
=	=	=	=	=	=	=	137->145	-0.3013
	27	Singlet-A	0.007	3.8497	322.06	31050.1		
=	=	=	=	=	=	=	126->139	-0.13008
=	=	=	=	=	=	=	132->140	0.169
=	=	=	=	=	=	=	133->140	0.14563
=	=	=	=	=	=	=	134->140	-0.10756
=	=	=	=	=	=	=	137->143	0.59886
=	=	=	=	=	=	=	137->144	-0.16571
=	=	=	=	=	=	=	137->145	0.13183
	28	Singlet-A	0.0209	3.854	321.7	31084.9		
=	=	=	=	=	=	=	132->140	-0.21711
=	=	=	=	=	=	=	133->140	-0.29314
=	=	=	=	=	=	=	137->143	0.25016
=	=	=	=	=	=	=	137->144	0.50865
=	=	=	=	=	=	=	137->145	0.13409
	29	Singlet-A	0.0011	3.8615	321.07	31145.9		
=	=	=	=	=	=	=	126->139	0.52011
=	=	=	=	=	=	=	132->140	0.12381
=	=	=	=	=	=	=	133->140	0.24378
=	=	=	=	=	=	=	137->144	0.21521
=	=	=	=	=	=	=	137->145	0.10376
=	=	=	=	=	=	=	138->147	-0.22304
	30	Singlet-A	0.03	3.8731	320.11	31239.3		
=	=	=	=	=	=	=	126->139	0.11221

=	=	=	=	=	=	132->140	-0.23417
=	=	=	=	=	=	133->140	-0.20418
=	=	=	=	=	=	137->144	-0.29317
=	=	=	=	=	=	137->145	0.50464
=	=	=	=	=	=	137->146	-0.15469

Corrole 5b in DMF

Coordinates:

C	1.72398	-4.21959	0.25754
C	2.91452	-3.4998	0.35323
C	2.67266	-2.176	-0.08022
C	0.73449	-3.35195	-0.23599
C	-0.68304	-3.34794	-0.27142
C	-2.63809	-2.22774	-0.18466
C	-2.92267	-3.61855	-0.09672
C	-1.71648	-4.30633	-0.1509
C	3.45128	-0.98985	-0.03487
C	2.85605	0.28194	-0.08621
C	3.48544	1.5519	-0.27136
C	2.52252	2.52715	-0.27137
C	1.24483	1.90552	-0.10463
C	-0.02247	2.50107	-0.05137
C	-1.26348	1.81015	0.01046
C	-2.55375	2.46972	-0.0214
C	-3.49755	1.49075	-0.00771
C	-2.79161	0.22917	0.02592
C	-3.40344	-1.04531	-0.03227
N	1.35157	-2.14454	-0.45459
H	0.98964	-1.44493	-1.08794
N	-1.28722	-2.13039	-0.3292
N	-1.43241	0.46197	0.03998
N	1.4956	0.55426	-0.01665
H	0.79581	-0.06452	0.36943
H	-2.71623	3.53813	-0.06748
H	-4.5713	1.6137	-0.05646
H	-3.90629	-4.05327	0.01722
H	-1.57746	-5.37842	-0.10816
H	1.55614	-5.23547	0.58956
H	3.8484	-3.85667	0.76567

H	4.5468	1.69154	-0.42258
H	2.67802	3.58825	-0.40561
C	4.91562	-1.11478	0.10991
C	5.6303	-2.0364	-0.67179
C	5.62661	-0.34063	1.04042
C	7.00778	-2.17148	-0.53453
H	5.09766	-2.63654	-1.40439
C	7.00496	-0.47322	1.17301
H	5.0866	0.35343	1.67838
C	7.7018	-1.38851	0.38626
H	7.54189	-2.88558	-1.15557
H	7.53447	0.13251	1.90348
H	8.77796	-1.49348	0.49256
C	-4.87213	-1.17774	0.08155
C	-5.59403	-1.94093	-0.84904
C	-5.57632	-0.56841	1.13127
C	-6.97362	-2.08335	-0.73775
H	-5.06625	-2.40783	-1.67629
C	-6.95619	-0.70986	1.2407
H	-5.02891	0.00367	1.8752
C	-7.66049	-1.46748	0.30683
H	-7.51443	-2.67152	-1.47432
H	-7.48141	-0.23399	2.06452
H	-8.73782	-1.57879	0.39364
C	-0.05982	3.9922	-0.09178
C	-0.49765	4.72546	1.01856
C	0.33827	4.69136	-1.23825
C	-0.5363	6.11691	0.98403
H	-0.80596	4.19527	1.91602
C	0.30423	6.08336	-1.27277
H	0.66842	4.1348	-2.11177
C	-0.13372	6.80071	-0.16159
H	-0.87712	6.66794	1.85663
H	0.61427	6.60731	-2.17305
H	-0.16237	7.88662	-0.18845
H	-0.87847	-1.19053	-0.23365

Frequencies:

		1	2	3
Frequencies	--	21.2902	32.0763	40.0071

TDDFT:

Order	Symm	f	Energy_eV	Energy_nm	Energy_cm-1	Transition	Coef
1	Singlet-A	0.3627	2.0488	605.15	16524.8		
=	=	=	=	=	=	137->139	0.10457
=	=	=	=	=	=	137->140	0.24461
=	=	=	=	=	=	138->139	0.64204
=	=	=	=	=	=	138->140	-0.12642
2	Singlet-A	0.033	2.1844	567.6	17618		
=	=	=	=	=	=	137->139	-0.45553
=	=	=	=	=	=	138->139	0.15499
=	=	=	=	=	=	138->140	0.50817
3	Singlet-A	0.8333	2.8645	432.82	23104.3		
=	=	=	=	=	=	135->139	-0.107
=	=	=	=	=	=	137->139	0.49204
=	=	=	=	=	=	137->140	0.11187
=	=	=	=	=	=	138->140	0.43574
=	=	=	=	=	=	138->141	-0.1296
4	Singlet-A	0.751	2.9743	416.85	23989.4		
=	=	=	=	=	=	136->139	0.37608
=	=	=	=	=	=	137->140	0.53098
=	=	=	=	=	=	138->139	-0.20075
5	Singlet-A	0.4791	3.0277	409.51	24419.4		
=	=	=	=	=	=	136->139	0.58589
=	=	=	=	=	=	137->140	-0.32552
=	=	=	=	=	=	138->139	0.1274
6	Singlet-A	0.1022	3.2476	381.77	26193.8		
=	=	=	=	=	=	134->139	-0.2253
=	=	=	=	=	=	135->139	0.60266
=	=	=	=	=	=	138->140	0.10745
=	=	=	=	=	=	138->141	0.21478
7	Singlet-A	0.0414	3.3319	372.11	26873.8		
=	=	=	=	=	=	134->139	0.60736
=	=	=	=	=	=	138->141	0.28232
8	Singlet-A	0.0025	3.4004	364.62	27425.8		
=	=	=	=	=	=	130->139	-0.14857
=	=	=	=	=	=	135->139	0.12312
=	=	=	=	=	=	138->141	-0.28877
=	=	=	=	=	=	138->142	0.58365
9	Singlet-A	0.006	3.4239	362.11	27615.9		
=	=	=	=	=	=	131->139	-0.18073
=	=	=	=	=	=	132->139	0.18353
=	=	=	=	=	=	138->141	0.1519

=	=	=	=	=	=	138->143	0.56695
=	=	=	=	=	=	138->145	-0.24486
10	Singlet-A	0.0035	3.4278	361.71	27646.5		
=	=	=	=	=	=	130->139	0.20946
=	=	=	=	=	=	131->139	0.12757
=	=	=	=	=	=	132->139	0.34762
=	=	=	=	=	=	133->139	0.38398
=	=	=	=	=	=	138->144	-0.38166
11	Singlet-A	0.0069	3.4305	361.42	27668.6		
=	=	=	=	=	=	129->139	0.16965
=	=	=	=	=	=	131->139	0.21968
=	=	=	=	=	=	132->139	0.22225
=	=	=	=	=	=	134->139	-0.13789
=	=	=	=	=	=	135->139	-0.13206
=	=	=	=	=	=	138->141	0.32763
=	=	=	=	=	=	138->142	0.21254
=	=	=	=	=	=	138->143	-0.1518
=	=	=	=	=	=	138->144	0.36028
12	Singlet-A	0.0123	3.4423	360.18	27763.9		
=	=	=	=	=	=	130->139	-0.11817
=	=	=	=	=	=	131->139	0.19403
=	=	=	=	=	=	136->140	-0.1675
=	=	=	=	=	=	138->143	0.26974
=	=	=	=	=	=	138->145	0.56272
=	=	=	=	=	=	138->146	-0.10819
13	Singlet-A	0.0059	3.4516	359.2	27839.6		
=	=	=	=	=	=	133->139	0.42401
=	=	=	=	=	=	134->139	0.14788
=	=	=	=	=	=	135->139	0.16183
=	=	=	=	=	=	138->141	-0.18794
=	=	=	=	=	=	138->142	-0.21145
=	=	=	=	=	=	138->143	0.11836
=	=	=	=	=	=	138->144	0.37369
14	Singlet-A	0.0405	3.4775	356.54	28047.3		
=	=	=	=	=	=	131->139	0.2512
=	=	=	=	=	=	133->139	0.13469
=	=	=	=	=	=	136->140	0.52481
=	=	=	=	=	=	138->146	-0.31252
15	Singlet-A	0.0117	3.4993	354.31	28223.9		
=	=	=	=	=	=	129->139	-0.16757
=	=	=	=	=	=	130->139	-0.14008
=	=	=	=	=	=	131->139	0.49007
=	=	=	=	=	=	132->139	-0.14386

=	=	=	=	=	=	136->140	-0.13001
=	=	=	=	=	=	138->143	0.11563
=	=	=	=	=	=	138->144	-0.1023
=	=	=	=	=	=	138->145	-0.26824
=	=	=	=	=	=	138->146	0.2496
16	Singlet-A	0.0313	3.5126	352.97	28331		
=	=	=	=	=	=	129->139	-0.16014
=	=	=	=	=	=	130->139	-0.26835
=	=	=	=	=	=	132->139	0.33289
=	=	=	=	=	=	136->140	0.31087
=	=	=	=	=	=	138->142	-0.11596
=	=	=	=	=	=	138->146	0.36137
17	Singlet-A	0.0139	3.5293	351.3	28465.7		
=	=	=	=	=	=	129->139	-0.19101
=	=	=	=	=	=	130->139	0.55053
=	=	=	=	=	=	133->139	-0.13775
=	=	=	=	=	=	136->140	0.11185
=	=	=	=	=	=	138->142	0.10364
=	=	=	=	=	=	138->143	0.1271
=	=	=	=	=	=	138->144	0.15631
=	=	=	=	=	=	138->146	0.16002
18	Singlet-A	0.0018	3.5465	349.6	28604.1		
=	=	=	=	=	=	128->139	0.16596
=	=	=	=	=	=	129->139	0.16142
=	=	=	=	=	=	131->139	0.17001
=	=	=	=	=	=	132->139	0.33666
=	=	=	=	=	=	133->139	-0.26583
=	=	=	=	=	=	135->139	0.1228
=	=	=	=	=	=	138->141	-0.23284
=	=	=	=	=	=	138->142	-0.14624
=	=	=	=	=	=	138->144	0.10348
=	=	=	=	=	=	138->145	-0.1066
=	=	=	=	=	=	138->146	-0.25419
19	Singlet-A	0.0119	3.6227	342.25	29218.4		
=	=	=	=	=	=	129->139	-0.41448
=	=	=	=	=	=	135->140	0.45177
=	=	=	=	=	=	137->141	0.19064
=	=	=	=	=	=	138->146	-0.1699
20	Singlet-A	0.0253	3.674	337.47	29632.3		
=	=	=	=	=	=	128->139	0.55872
=	=	=	=	=	=	129->139	0.14651
=	=	=	=	=	=	132->139	-0.13431
=	=	=	=	=	=	133->139	0.12503

=	=	=	=	=	=	135->140	0.27386
=	=	=	=	=	=	138->147	-0.11323
21	Singlet-A	0.0196	3.7322	332.2	30102.3		
=	=	=	=	=	=	128->139	-0.22928
=	=	=	=	=	=	129->139	0.22589
=	=	=	=	=	=	134->140	-0.28913
=	=	=	=	=	=	135->140	0.36048
=	=	=	=	=	=	137->141	-0.26209
=	=	=	=	=	=	138->146	0.122
=	=	=	=	=	=	138->147	0.1741
22	Singlet-A	0.0409	3.7728	328.63	30429.4		
=	=	=	=	=	=	128->139	-0.1373
=	=	=	=	=	=	129->139	0.10286
=	=	=	=	=	=	134->140	0.54381
=	=	=	=	=	=	135->140	0.13088
=	=	=	=	=	=	137->141	-0.26486
=	=	=	=	=	=	138->147	-0.20853
23	Singlet-A	0.0178	3.7915	327	30581		
=	=	=	=	=	=	127->139	0.62231
=	=	=	=	=	=	133->140	0.14447
=	=	=	=	=	=	134->140	0.16246
=	=	=	=	=	=	138->147	0.12485
24	Singlet-A	0.0035	3.8116	325.28	30742.7		
=	=	=	=	=	=	126->139	-0.17436
=	=	=	=	=	=	128->139	0.10616
=	=	=	=	=	=	129->139	-0.10907
=	=	=	=	=	=	130->140	0.10587
=	=	=	=	=	=	133->140	0.17631
=	=	=	=	=	=	137->141	-0.2581
=	=	=	=	=	=	137->142	0.40368
=	=	=	=	=	=	138->147	0.34351
25	Singlet-A	0.0291	3.8224	324.36	30829.9		
=	=	=	=	=	=	126->139	-0.32113
=	=	=	=	=	=	127->139	-0.12393
=	=	=	=	=	=	132->140	-0.13012
=	=	=	=	=	=	134->140	0.17032
=	=	=	=	=	=	137->141	0.23125
=	=	=	=	=	=	137->142	-0.27159
=	=	=	=	=	=	137->143	-0.12409
=	=	=	=	=	=	137->144	-0.14724
=	=	=	=	=	=	138->147	0.34072
26	Singlet-A	0.0026	3.8463	322.35	31022.2		
=	=	=	=	=	=	126->139	-0.13805

=	=	=	=	=	=	127->139	0.1221
=	=	=	=	=	=	130->140	-0.10242
=	=	=	=	=	=	132->140	-0.10735
=	=	=	=	=	=	133->140	-0.15231
=	=	=	=	=	=	137->141	0.24901
=	=	=	=	=	=	137->142	0.46567
=	=	=	=	=	=	137->144	-0.16554
=	=	=	=	=	=	137->145	-0.2585
27	Singlet-A	0.0016	3.8515	321.91	31064.6		
=	=	=	=	=	=	126->139	-0.16726
=	=	=	=	=	=	132->140	0.31442
=	=	=	=	=	=	133->140	0.41582
=	=	=	=	=	=	137->143	-0.14703
=	=	=	=	=	=	137->144	-0.34565
=	=	=	=	=	=	138->147	-0.14807
28	Singlet-A	0.0085	3.8542	321.69	31085.8		
=	=	=	=	=	=	126->139	-0.32078
=	=	=	=	=	=	133->140	0.12064
=	=	=	=	=	=	137->143	0.57447
=	=	=	=	=	=	137->144	0.13996
29	Singlet-A	0.0104	3.8589	321.29	31124.5		
=	=	=	=	=	=	126->139	0.37052
=	=	=	=	=	=	127->139	-0.10054
=	=	=	=	=	=	137->143	0.32034
=	=	=	=	=	=	137->144	-0.36545
=	=	=	=	=	=	137->145	-0.19933
=	=	=	=	=	=	138->147	0.19977
30	Singlet-A	0.0378	3.8749	319.97	31252.9		
=	=	=	=	=	=	132->140	-0.20296
=	=	=	=	=	=	133->140	-0.14445
=	=	=	=	=	=	137->143	0.10018
=	=	=	=	=	=	137->144	-0.35262
=	=	=	=	=	=	137->145	0.50456
=	=	=	=	=	=	137->146	-0.15034