Electronic Supplementary Information

Spin Multiplicity Effects in Doublet versus Singlet Emission: The Photophysical Consequences of a Single Electron

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Contents for Supporting Information:

I. Steady State Spectroscopy

Both **DC** and **RC** were synthesized according to the procedure previously reported in the literature. (S1) ***No unexpected or unusually high safety hazards were encountered.***

UV-Vis-NIR spectral data were measured at room temperature (298 K) with a Varian Cary 5000 spectrophotometer. All solvents used for solution samples were dried and degassed before use. Wavelengths are shown in nanometers (nm), and absorption in arbitrary units (a. u.).

Fluorescence data were measured at room temperature (298 K) with a HORIBA Fluorolog-3 spectrofluorometer. All solvents used for solution samples were dried and degassed prior to use. Wavelengths are shown in nanometers (nm), and fluorescence is reported in arbitrary units (arb. units). Relative photoluminescence quantum yields were determined by cross-calibration with cresyl violet (0.56) and sulforhodamine 101 (0.95), and applying refractive index corrections. Lifetime measurements were determined using the time-correlated single photon counting (TCSPC) technique, where a nanoLED laser (478 nm) was used as an excitation source. Lifetimes were calculated using Horiba DAS6 Fluorescence decay analysis software.

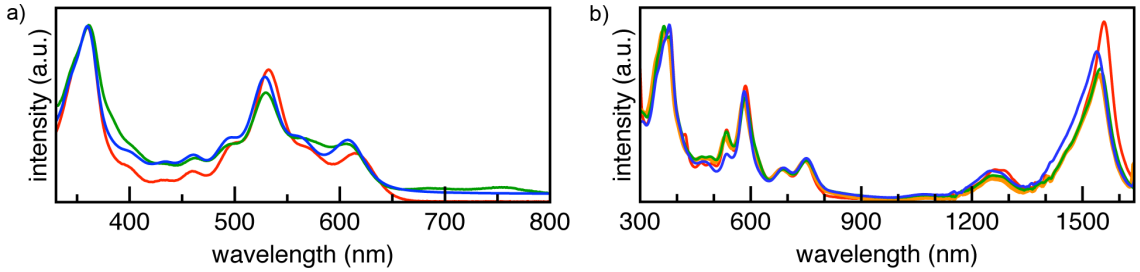


Figure S1. Absorption spectra for **DC** (a) in ethyl acetate (red), acetone (green), and acetonitrile (ACN, blue). Absorption spectra for **RC** (b) are measured in dichloromethane (DCM, red), 2:1 DCM:ACN (orange), 1:1 DCM:ACN (green), ACN (blue).

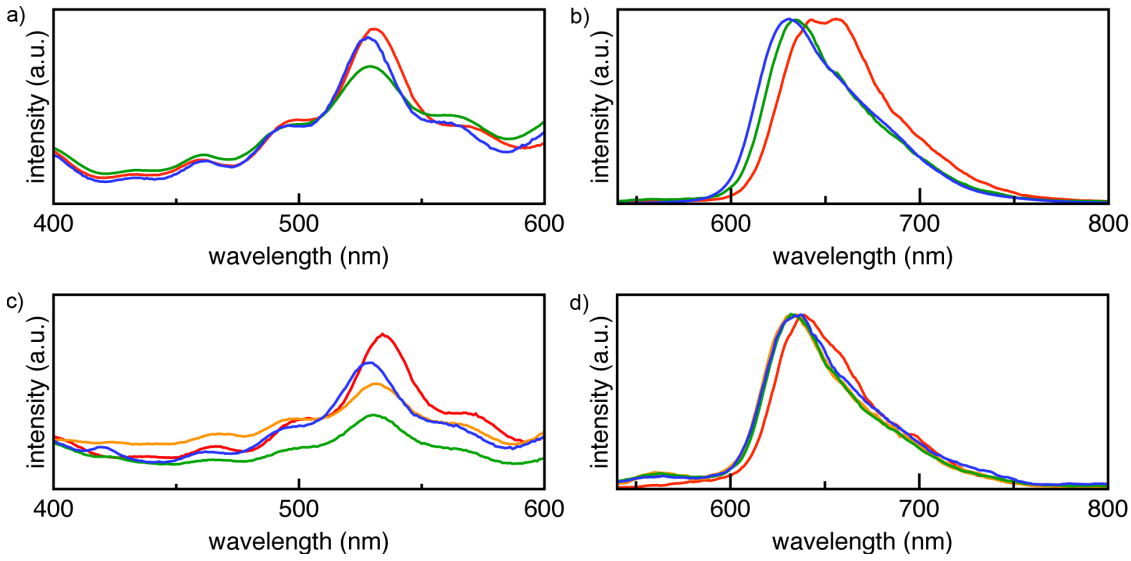


Figure S2. Excitation (a) and emission (b) spectra for **DC** in ethyl acetate (red), acetone (green), and acetonitrile (ACN, blue). Excitation (c) and emission (d) spectra for **RC** are measured in dichloromethane (DCM, red), 2:1 DCM:ACN (orange), 1:1 DCM:ACN (green), ACN (blue).

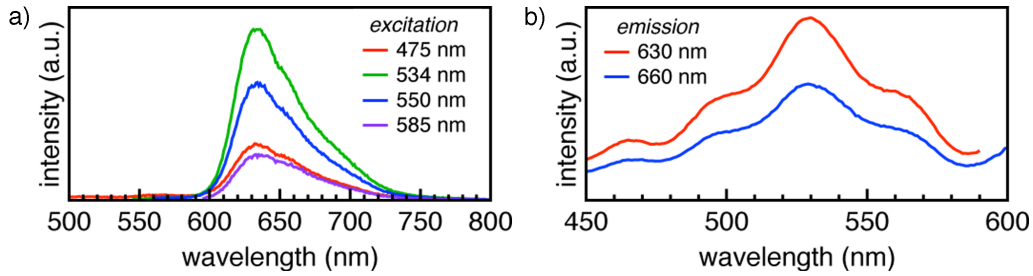


Figure S3. Emission spectra for **RC** (a) upon excitation at varying wavelengths, ranging from 475-585 nm. Photoluminescence excitation spectra for **RC** (b) that correspond to different emission wavelengths (PL λ_{max}). Both sets of data were collected from ACN solutions.

Singlet O_2 Detection Experiments

The **DC** solution (6.25 x 10^{-5} M) was prepared in ACN saturated with O_2 by bubbling pure O_2 for 30 min. A Fluorolog spectrofluorometer equipped with a Xe lamp (450W), single-grating monochromators, and NIR accessories was used for $^1O_2$ detection. The **DC** sample was excited at 535 nm with a bandpass (5 nm) filter. NIR detector (DSS-IGA020L InGaAs) was used to measure the emission spectrum of $^1O_2$ at liquid N_2 temperature. The emission spectrum was obtained with an integration time of 1 s and a bandpass of 12 nm using a long pass filter.

The **RC** solution (6.25 x 10^{-5} M) was prepared similarly in (DCM:ACN 2:5) saturated with O_2 by bubbling pure O_2 for 30 min. No emission peak was noted for $^1O_2$ even increasing the concentration of **RC** to 1.25 x 10^{-4} M.

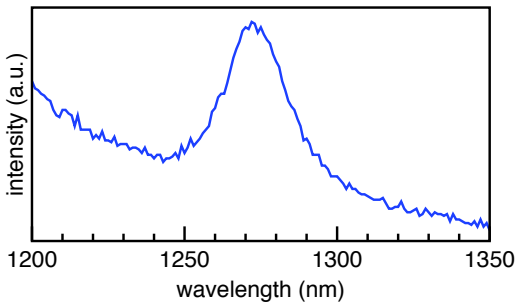


Figure S4. Fluorescence spectrum of singlet oxygen ($^1O_2$) formation upon irradiating (535 nm) **DC** in an O_2-saturated ACN solution.

II. Transient Absorption Spectroscopy

Transient absorption spectroscopy was performed with an Ultrafast Systems Helios/EOS spectrometer. Pulses of laser light of 150 fs duration and 800 nm wavelength were generated with a Coherent Libra amplified Ti:sapphire system at 1.3 W and 1 kHz repetition rate. Approximately 80% of the 800 nm pulses was sent to a Topas-C optical parametric amplifier to generate a 530 nm pump pulse. The pump pulse was passed through a depolarizing optic to eliminate contributions to the TA signal from orientational diffusion and was attenuated to 0.4−0.5 μJ/pulse. The excitation beam was focused to a spot size of ~2 mm to produce an excitation density of ~16 μJ/cm^2 per pulse. The remainder (~20 %) of the 800 nm light was sent through a sapphire crystal to generate a white light continuum for use as the probe pulse (for Helios, femtosecond TA). Referencing was accomplished by subtracting the ΔA spectrum calculated for the reference channel from the ΔA spectrum calculated for the probe channel, for each pump-on/pump-off pair of the probe pulses. The TA spectra were measured over a 5-ns window. For each scan, 250 time points were recorded with exponential time spacing, and each sample was subjected to three scans in addition to samples being prepared in triplicate. Data analysis was performed using global analysis software (Ultrafastsystems Surface Xplorer) by extracting and retaining 2-3 principal components and fitting to isolate DADS and their corresponding lifetimes. The number of principal components and DADS chosen when fitting the data set of each configuration was selected to obtain the lowest error value provided by the Surface Xplorer software (i.e. the value of χ^2 that was closest to 1). Quality of the fitting was also assessed by examining the residuals of the principle component kinetic traces. For nanosecond TA (EOS mode), the pump pulses were the same as those used for the Helios (femtosecond TA). The white light for the probe beam was generated using fiber optic laser (a pulsed PCF-based laser). Time delays are sampled randomly using an electronically controlled delay in the selected time window.

Sample for transient absorption were prepared in triplicate and stirred with a magnetic stir bar during every run. Samples were prepared in a nitrogen environment in a 2-mm quartz high-vacuum cuvette. The concentration of each sample was ~100 μM. UV-visible absorption spectra were recorded before and after each TA experiment to verify that no decomposition had occurred.

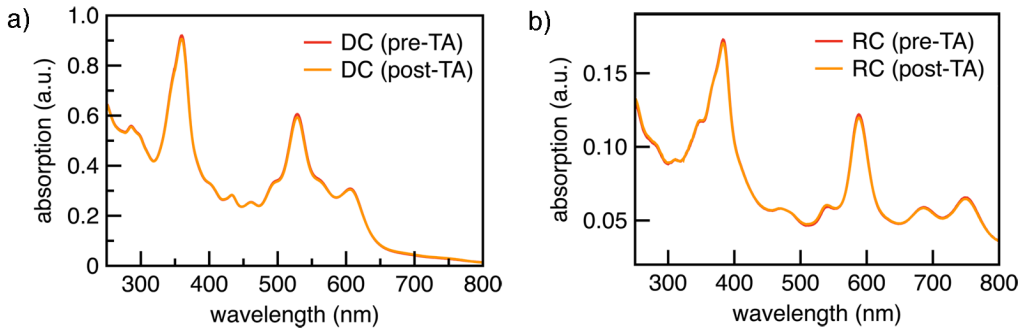


Figure S5. Steady-state absorption spectra of **DC** (a) and **RC** (b) taken before and after each TA experiment to verify that no decomposition had occurred. The absorption spectra pre- and post-TA are nearly coincident with each other.

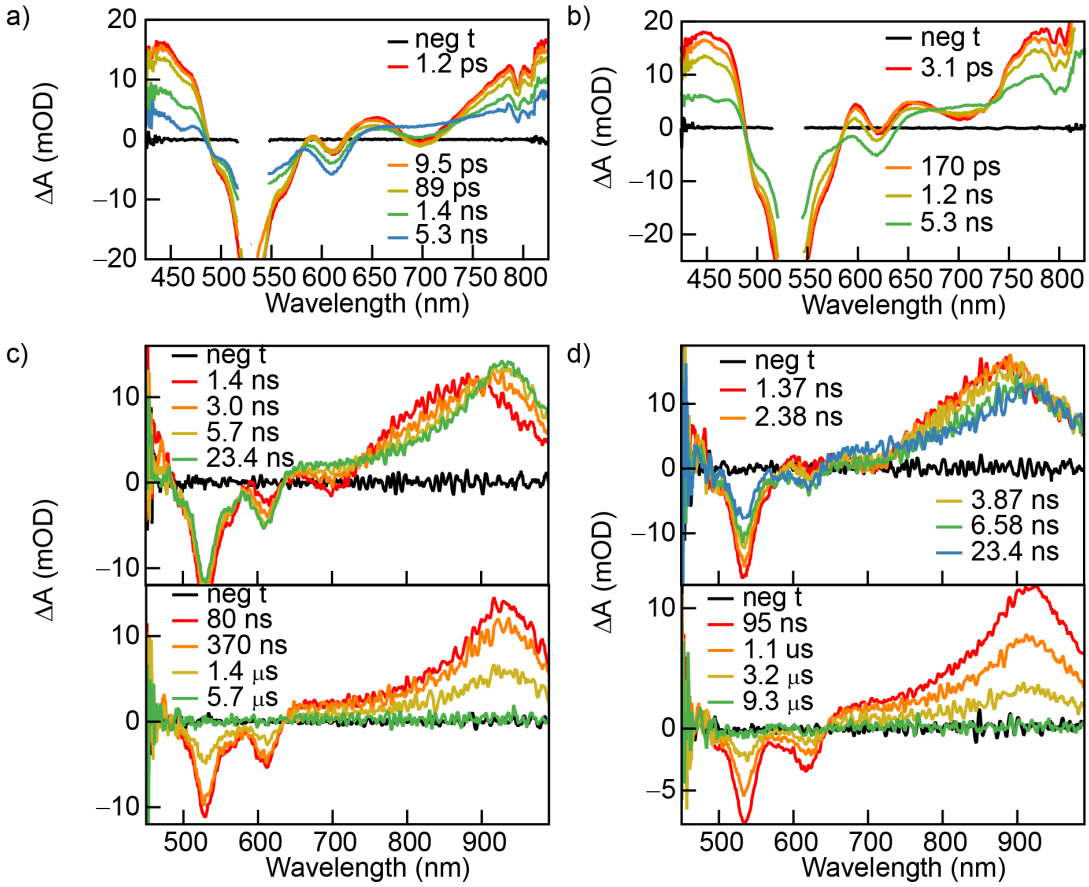


Figure S6. Transient absorption spectra of **DC** (a, c) acetone and (b, d) in ethlyacetate. a) and b) show kinetics from femtosecond TA spectra from 0 to 5 ns. c) and d) show nanosecond TA spectra over a range of time delays. Gaps in the spectra around 530 nm correspond to removal of scatter laser excitation light.

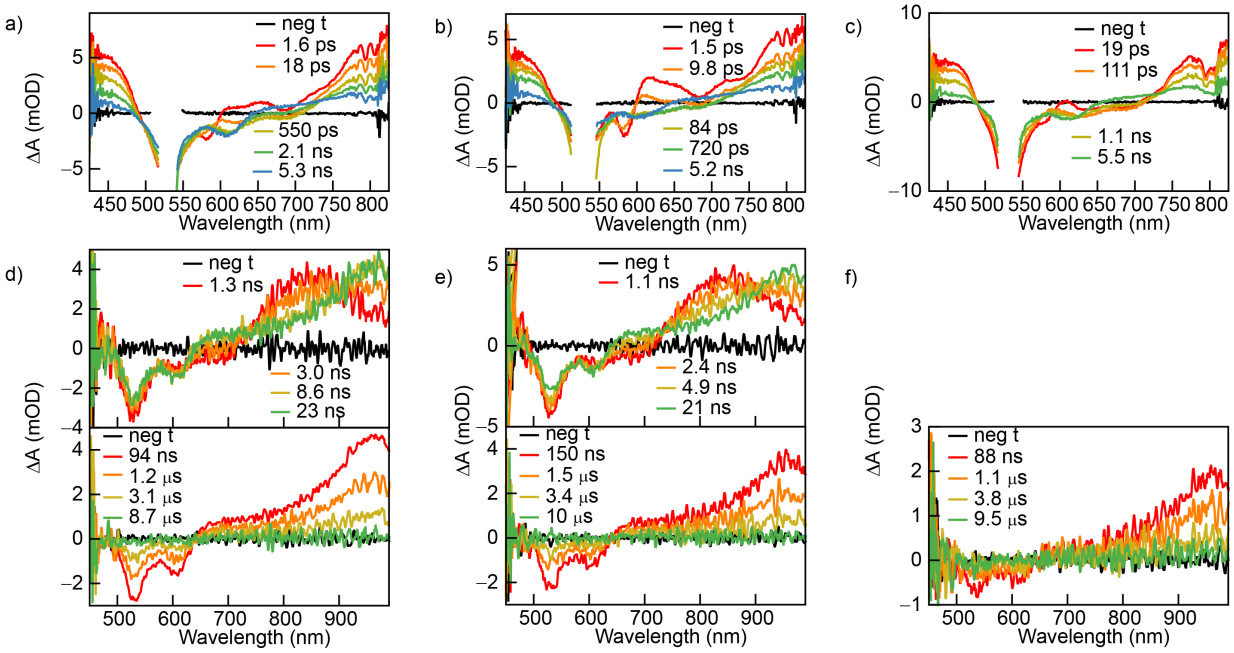


Figure S7. Transient absorption spectra of **RC** (a, d) 1:1 DCM:ACN, (b, e) 2:1 DCM:ACN and (c, f) dichlormethane (DCM). a), b) and c) show kinetics from femtosecond TA spectra from 0 to 5 ns. d), e) and f) show nanosecond TA spectra over a range of time delays. Gaps in the spectra around 530 nm correspond to removal of scatter laser excitation light.

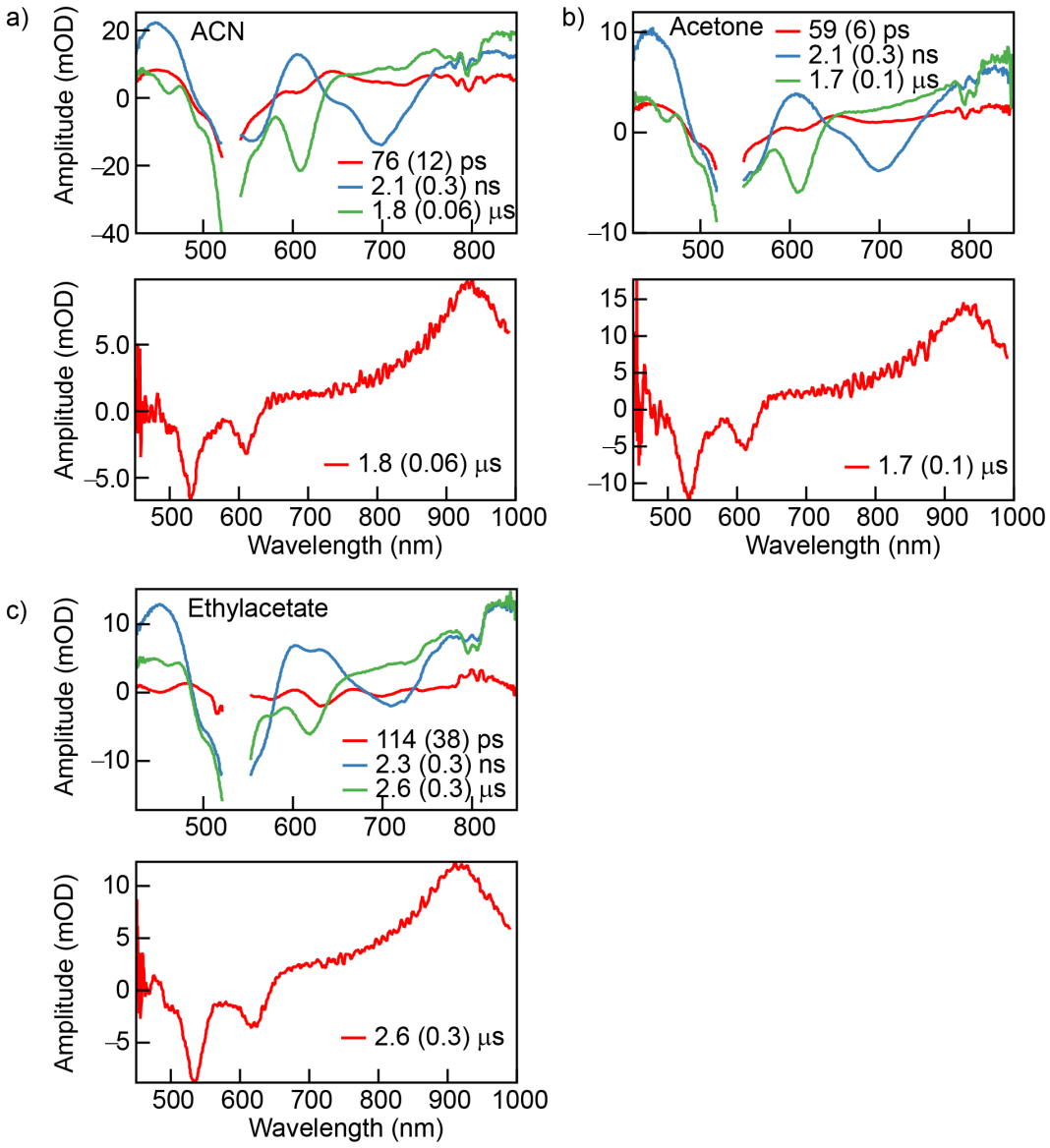


Figure S8. Global analysis decay-associated difference spectra (DADS) of **DC** in (a) acetonitrile, (b) acetone and (c) ethylacetate. Top tile shows DADS obtained from fitting fs TA data. Bottom tile shows the DADS obtained from ns TA data fitting. The longest lifetime DADS of fs TA fitting matches with the DADS obtained from ns TA data fitting indicating that these two species are the same. Note that the fs and ns DADS spectra are shown on different wavelength ranges. Gaps in the spectra around 530 nm correspond to removal of scatter laser excitation light.

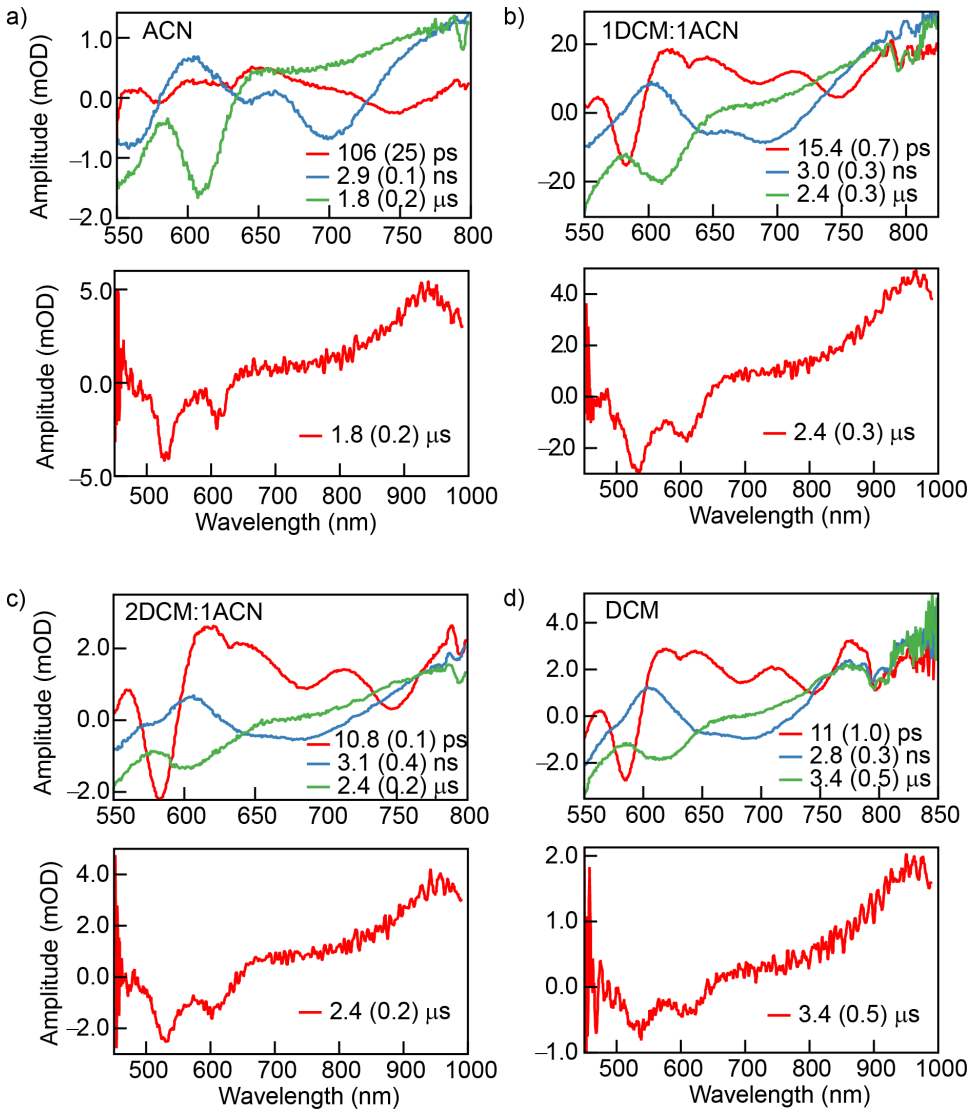


Figure S9. Global analysis decay-associated difference spectra (DADS) of **RC** in (a) acetonitrile, (b) 1:1 DCM:ACN (c) 2:1 DCM:ACN and (d) dichlormethane (DCM). Top tile shows DADS obtained from fitting fs TA data. Bottom tile shows the DADS obtained from ns TA data fitting. The longest lifetime DADS of fs TA fitting matches with the DADS obtained from ns TA data fitting indicating that these two species are the same. Note that the fs and ns DADS spectra are shown on different wavelength ranges. Gaps in the spectra around 530 nm correspond to removal of scatter laser excitation light.

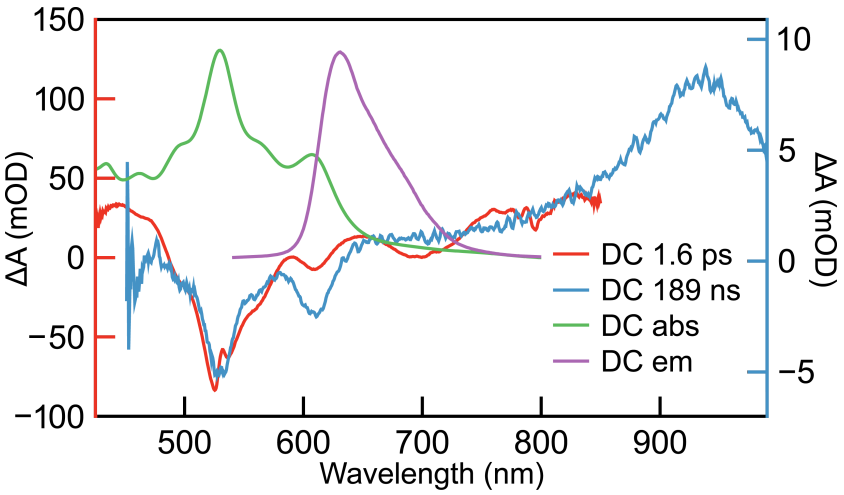


Figure S10. Transient absorption spectra of **DC** taken at 1.6 ps and 189 ns overlaid with steady-state absorption and emission (λ_{exc} = 530 nm) spectra.

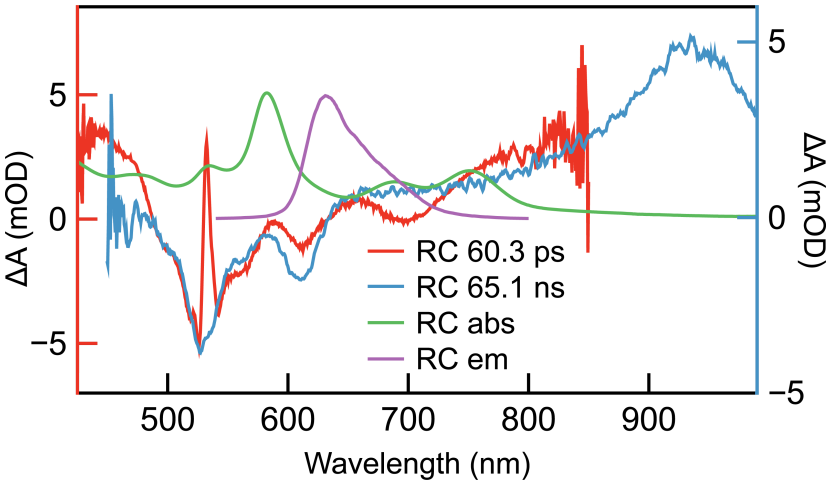


Figure S11. Transient absorption spectra of **RC** taken at 60.3 ps and 65.1 ns overlaid with steady-state absorption and emission (λ_{exc} = 530 nm) spectra.

III. Comparisons of Ground and Emissive Excited State Structures of DC and RC

All calculations were performed using the Gaussian09 program. (S3) The relaxed ground state geometries of **DC** and **RC** were optimized using a range of hybrid functionals with standard Gaussian type orbital (GTO) basis sets of double-ζ quality with polarization and dispersion, 6-31+G(d,p), with a complete polarizable continuum model (PCM) solvent description of acetonitrile. In addition, dispersion was accounted for using the GD3 correction. Each ground state was run with the known charge and multiplicity, **DC** +2 singlet and **RC** +1 doublet. Each singlet was checked for open-shell character through a stability check and each geometry was confirmed as a true minimum with no imaginary frequencies.

A. Comparisons of Energies

Table S1. DFT and TDDFT energies of relevant excited states at the optimized ground state, experimentally relevant excited state, and higher spin state for **DC** and **RC**.

	Geometry	State	Energy (eV)
DC	GS	S_0	0.00
	GS	S_1	2.07
	GS	S_2	2.35
	GS	S_3	2.55
	GS	S_4	2.77
	GS	T_1	1.44
	ES	S_2	2.77
	T_1	T_1	1.42
RC	GS	D_0	0.00
	GS	D_1	0.92
	GS	D_2	1.59
	GS	D_3	1.79
	GS	D_4	2.23
	GS	Q_1	2.00
	ES	D_4	2.00
	Q_1	Q_1	1.74

B. Comparisons of Molecular Geometries

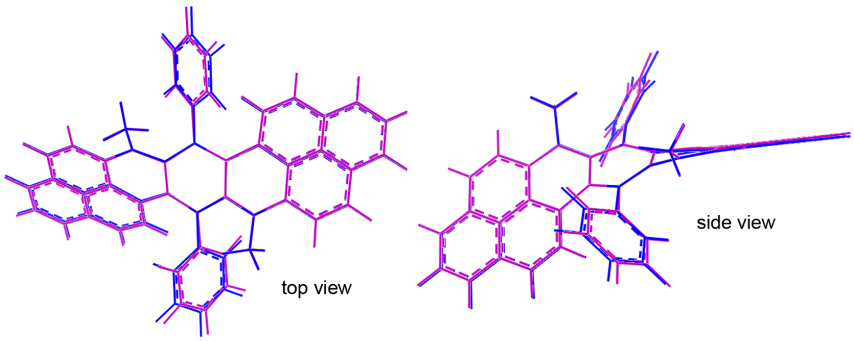


Figure S12. Comparison of optimized ground state (S_0, blue) and emissive excited state (S_2, excited state 2 in Table S6, pink) geometries of **DC**.

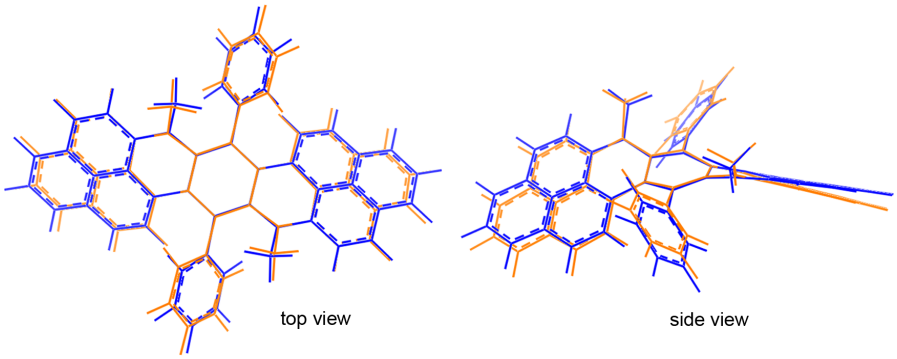


Figure S13. Comparison of optimized ground state (D_0, blue) and emissive excited state (D_4, excited state 5 in Table S17, orange) geometries of **RC**.

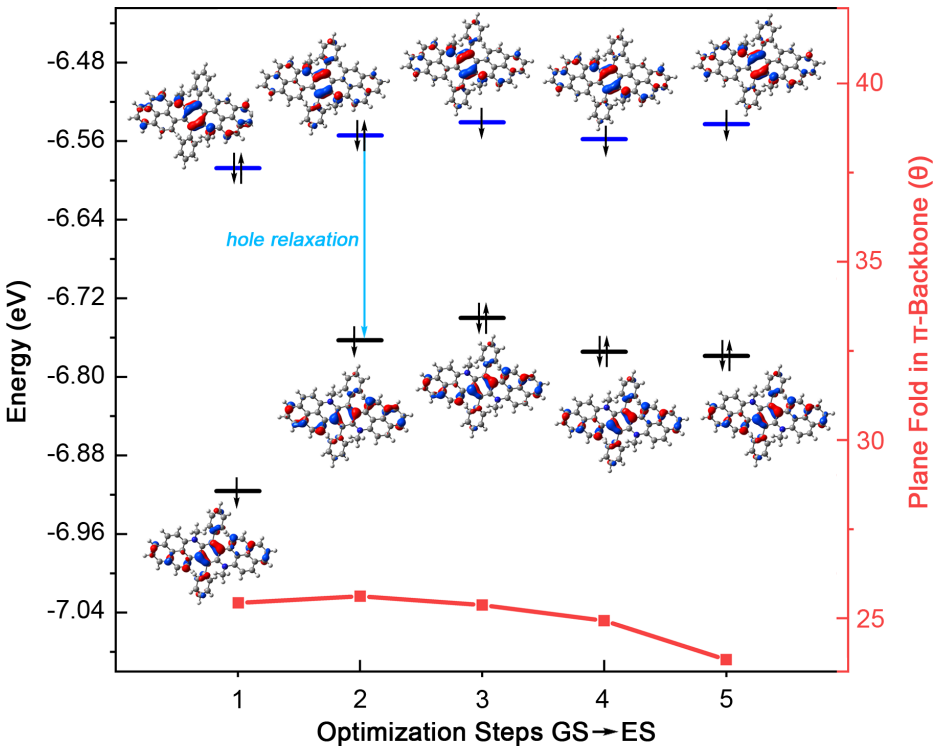


Figure S14. HOMO (blue) and HOMO-1 (black) energy levels of **DC** along the path of the TDDFT excited state geometry optimization of S_2 from the ground state (excited state 2 in Table S6) to ES (S_2). Changes to the curvature (red) of the π-backbone are also shown.

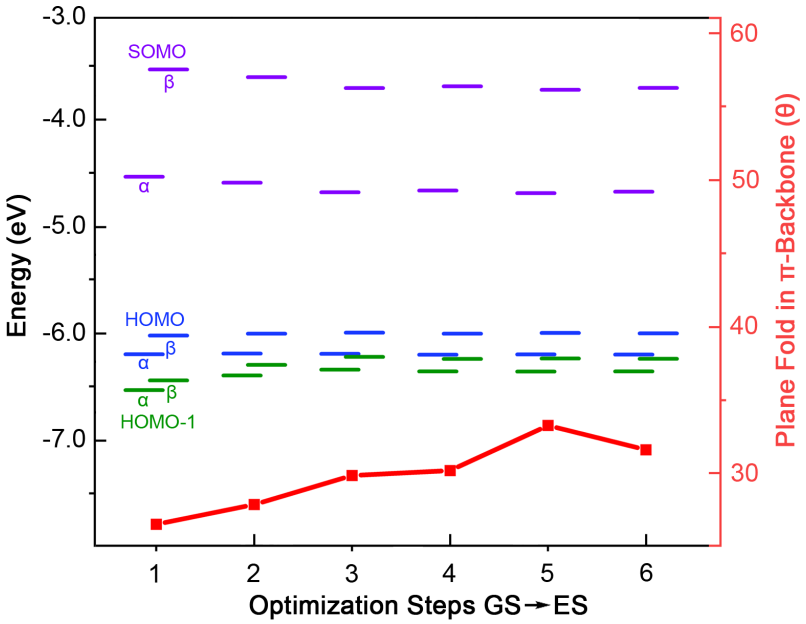


Figure S15. SOMO (purple), HOMO (blue), and HOMO-1 (green) energy levels of **RC** along the path of the TDDFT excited state geometry optimization of D_4 from the ground state (excited state 5 in Table S17) to ES (D_4). Changes to the curvature (red) of the π-backbone are also shown.

C. Comparisons of Electronic Structures

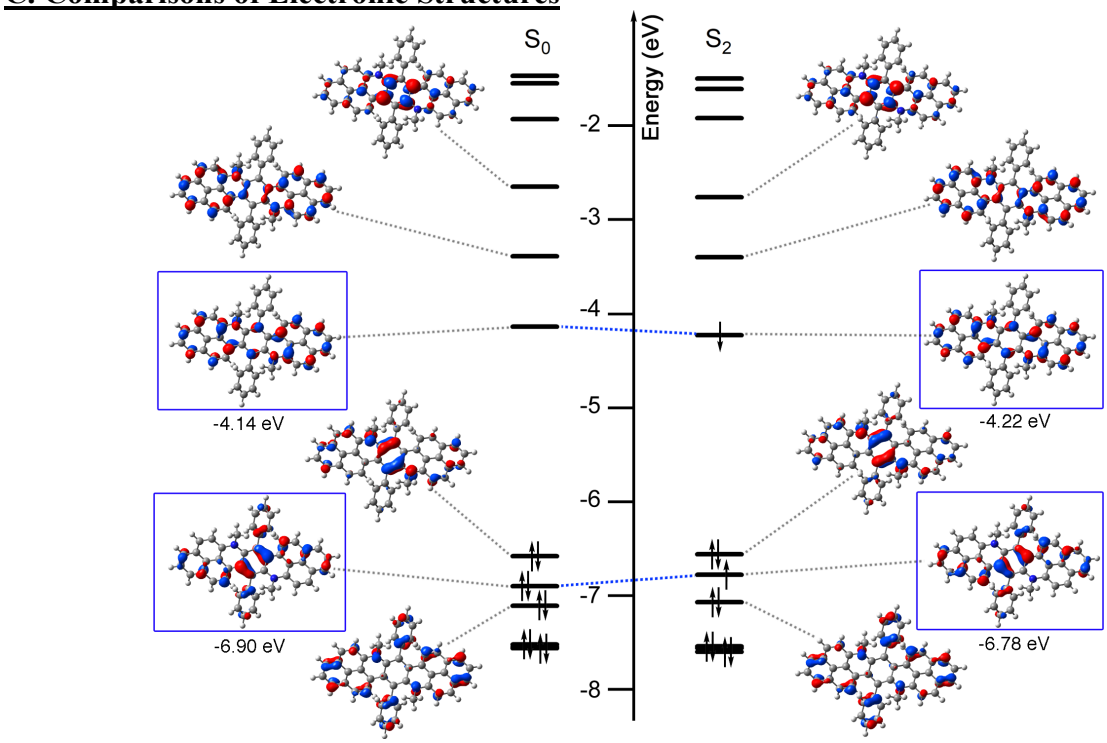


Figure S16. Calculated molecular orbital diagrams of **DC** in the optimized ground state and emissive excited state (S_2, excited state 2 in Table S6) geometries.

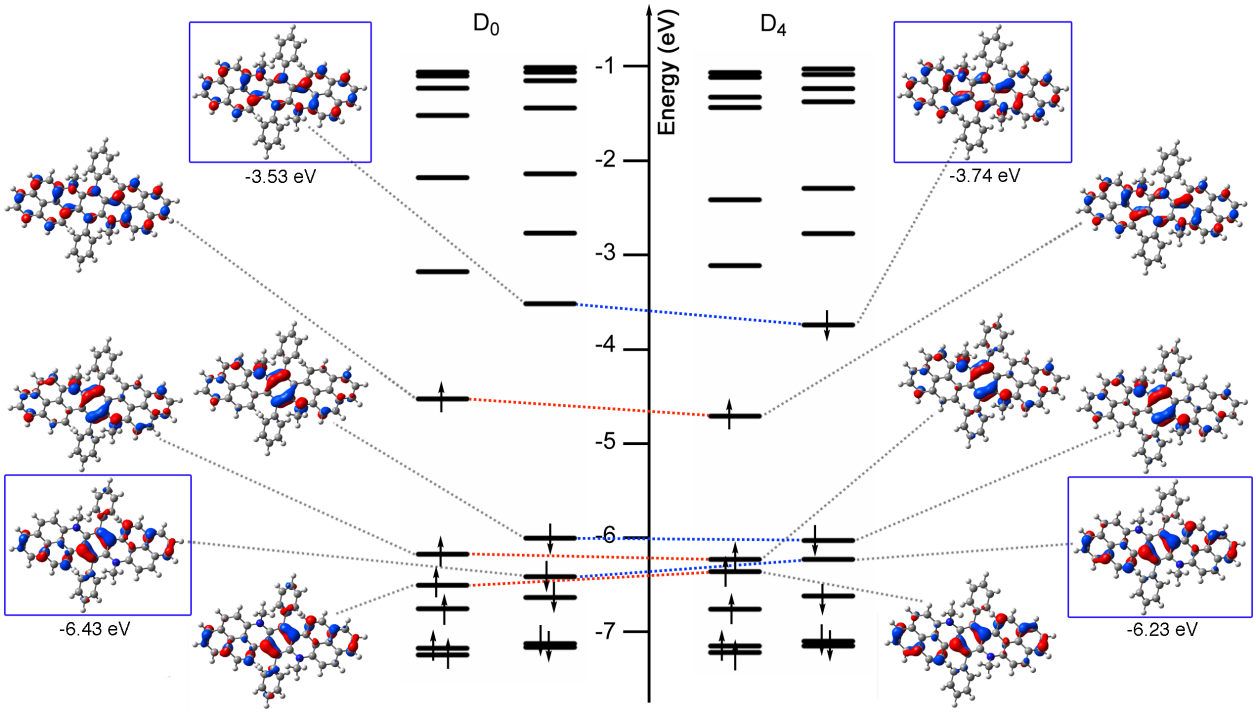


Figure S17. Calculated molecular orbital diagrams of **RC** in the optimized ground state and emissive excited state (D_4, excited state 5 in Table S17) geometries.

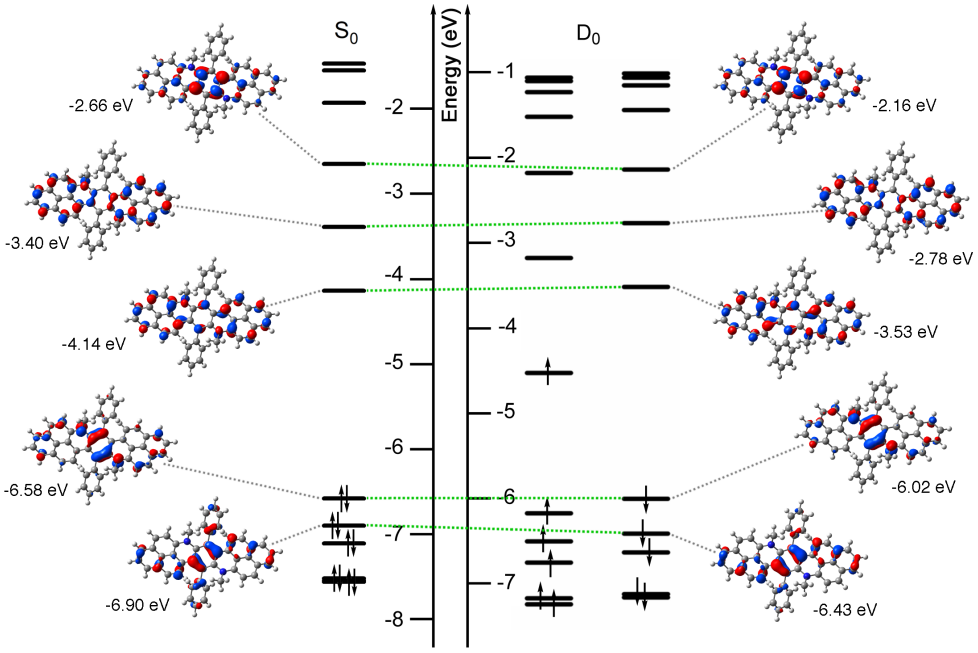


Figure S18. Aligned frontier molecular orbitals of the optimized ground states of **DC** and **RC**. Energy level spacings between the highest doubly-occupied and unoccupied molecular orbitals are extremely similar between **DC** and **RC**, which is in agreement with the observation that both species show near-identical transient absorption spectral features.

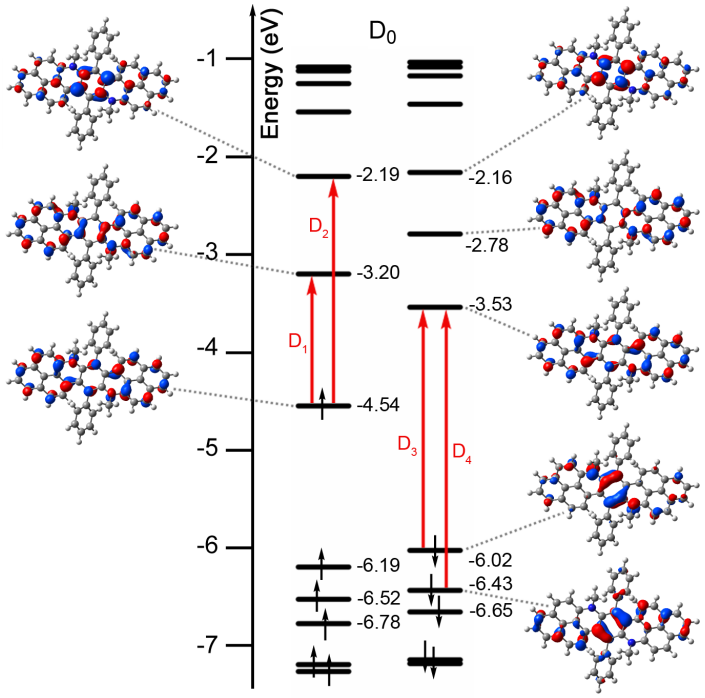


Figure S19. Calculated molecular orbital diagram of **RC** in the optimized ground state and the electronic transitions related to the formations of D_1, D_2, D_3 and D_4(Table S17).

D. Predicted Absorption Method Dependence

Figure S20. Absorption spectra calculated for **DC** by CIS or TDDFT with different functionals (a-h), including D3-B3LYP with the Tamm-Dancoff approximation (i), and a comparison of orbital energies based on functional (j).

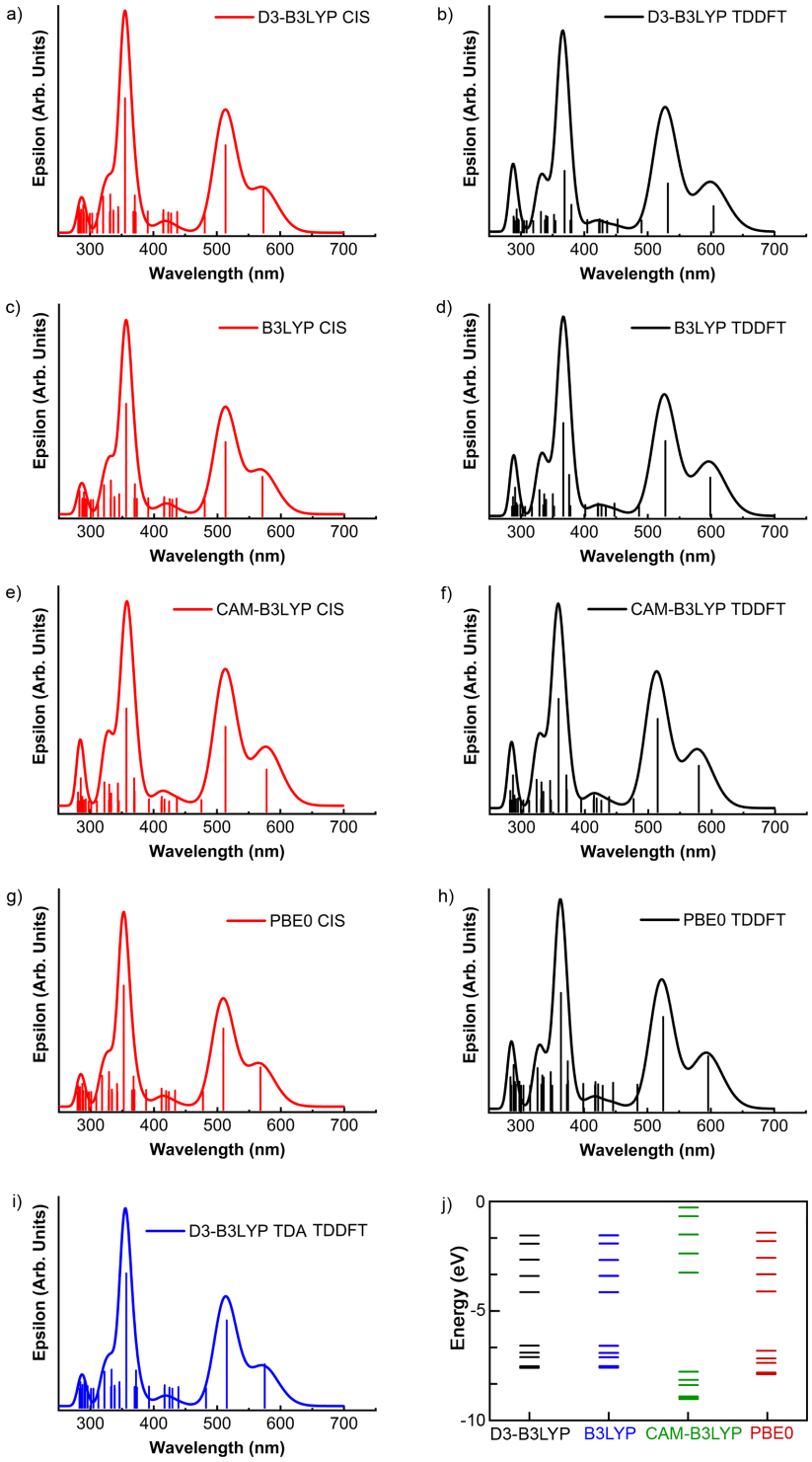
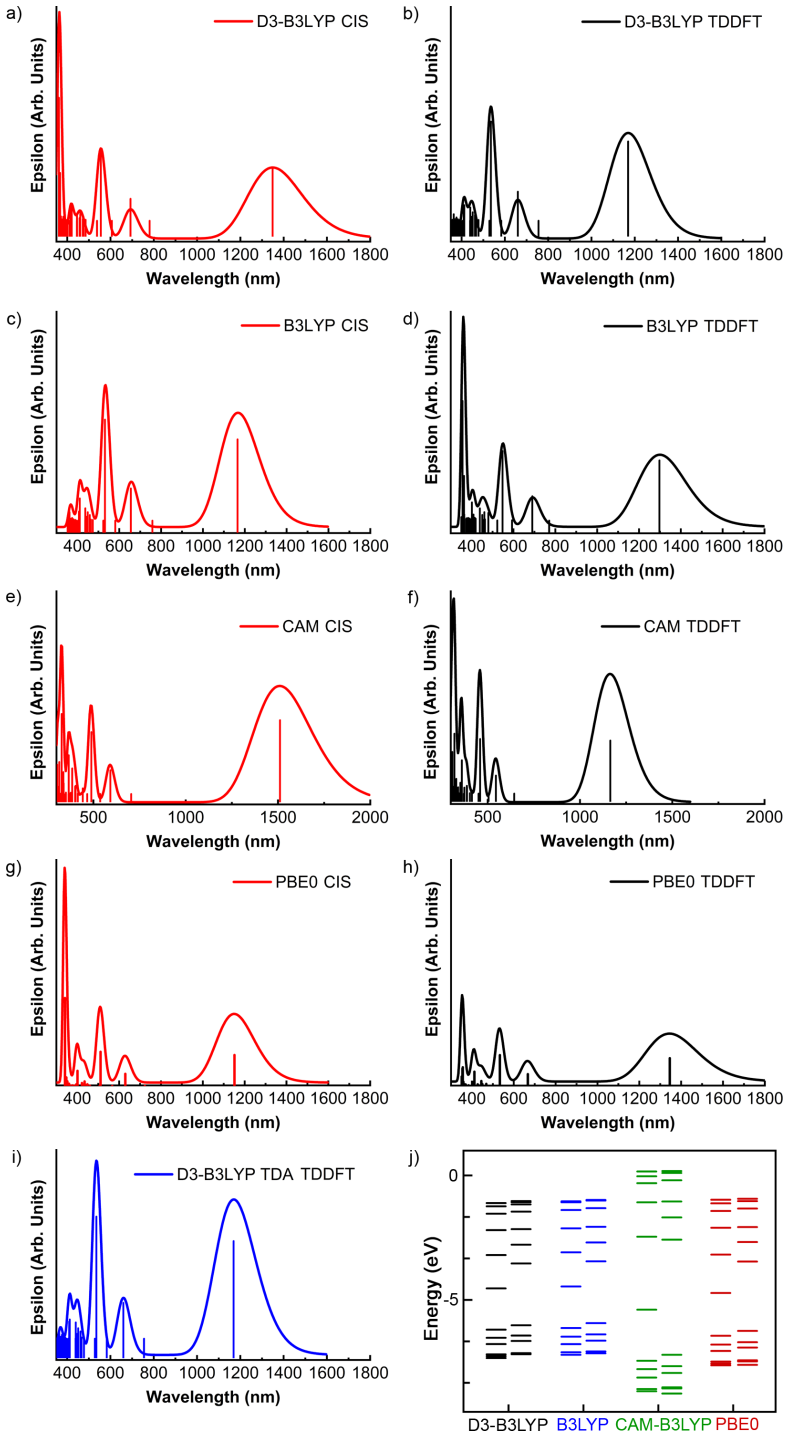


Figure S21. Absorption spectra calculated for **RC** by CIS or TDDFT with different functionals (a-h), including D3-B3LYP with the Tamm-Dancoff approximation (i), and a comparison of orbital energies based on functional (j).



IV. Vibrational Analyses

Table S2. Low frequency (< 100 cm^{-1}) molecular vibrations present in **DC**. Displacement vectors shown scaled by 1.

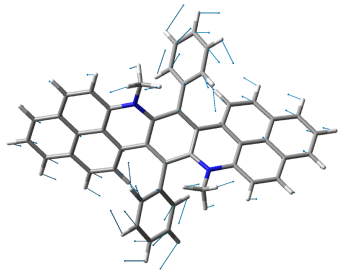
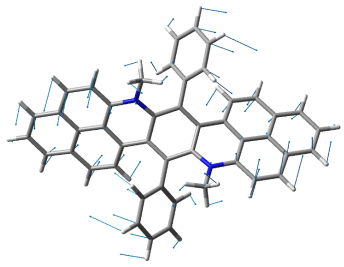
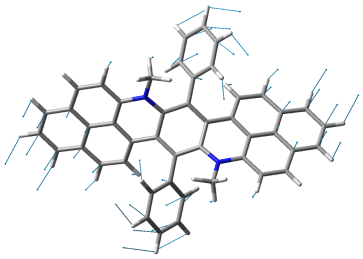
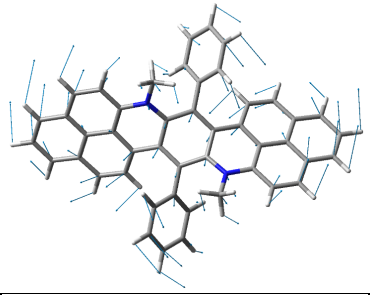
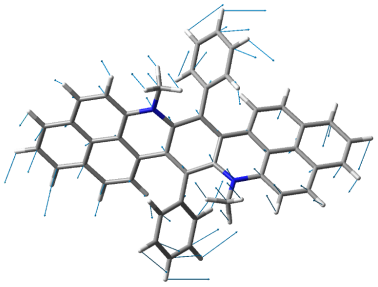
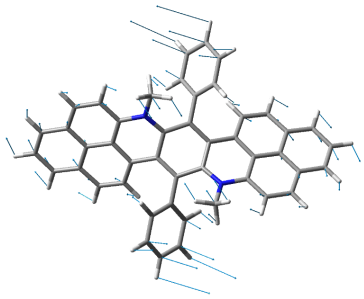
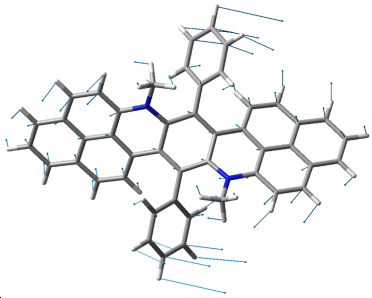
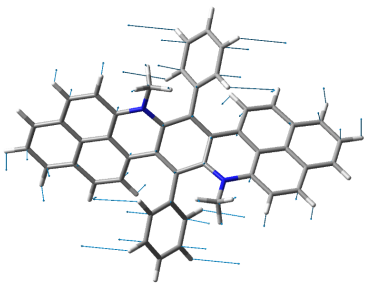
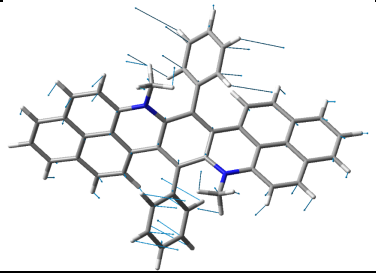
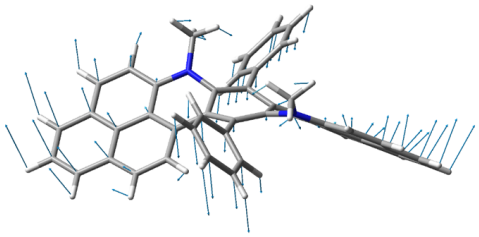
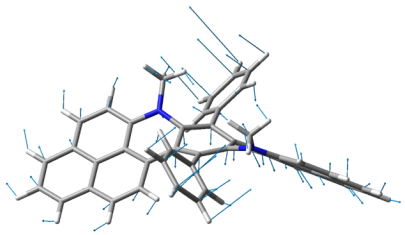
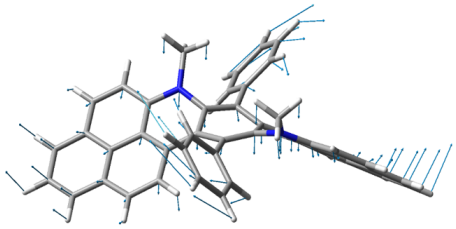
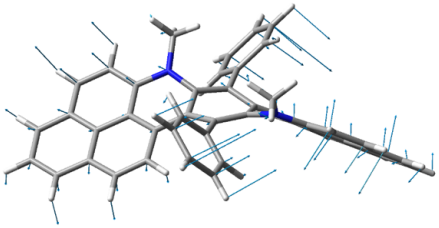
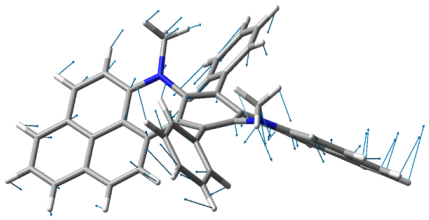
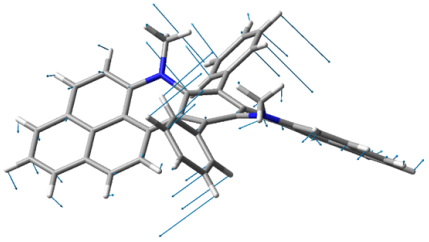
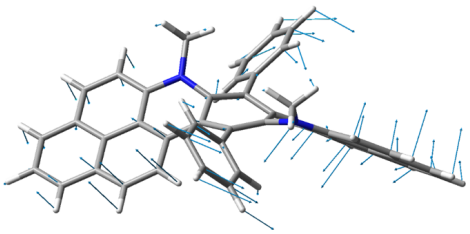
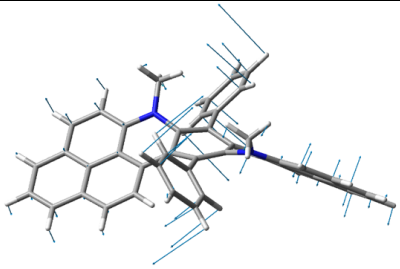
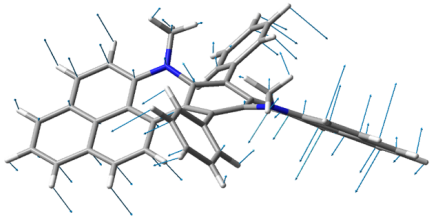
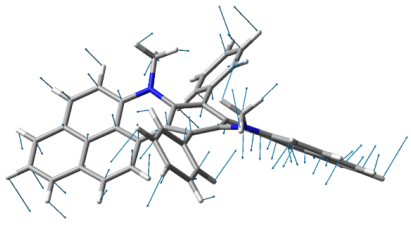
Frequency (cm^{-1})	Vector Displacement	Frequency (cm^{-1})	Vector Displacement
15.63		36.81	
30.29		40.91	
32.41		52.53	
56.73		88.81	
83.37			

Table S3. Low frequency (< 100 cm^{-1}) molecular vibrations present in **RC**. Displacement vectors shown scaled by 1.

Frequency (cm^{-1})	Vector Displacement	Frequency (cm^{-1})	Vector Displacement
20.64		56.35	
35.80		61.92	
40.30		81.02	
44.47		84.57	
45.23		94.66	

Vibrational modes within classical polycyclic aromatic hydrocarbons: an oxygen-embedded quinoidal pentacene (reference S2)

Ground state optimized geometry

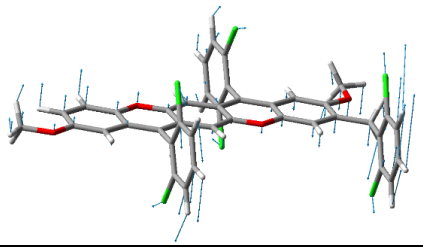
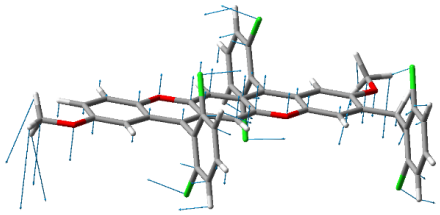
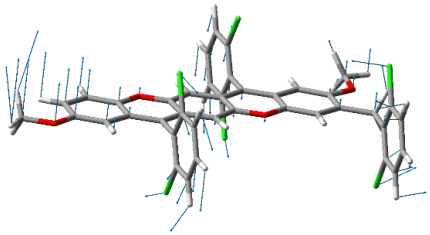
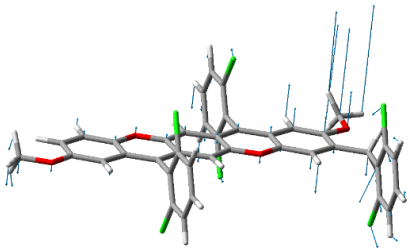
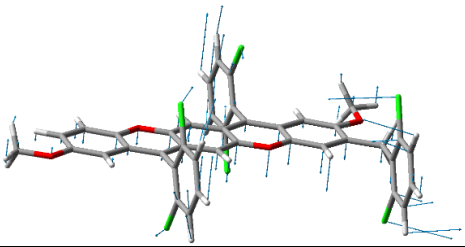
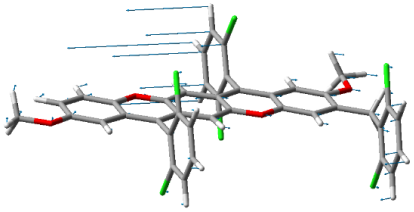
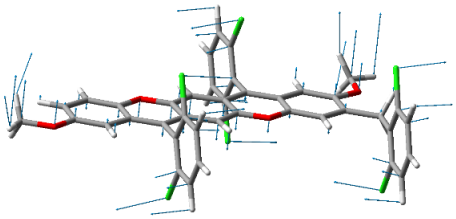
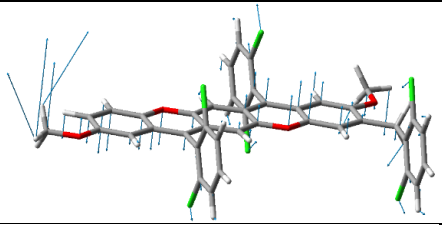
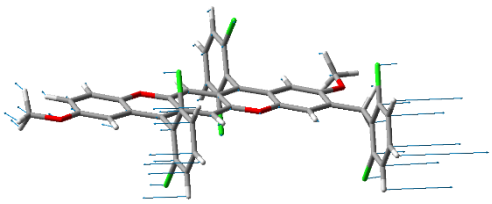
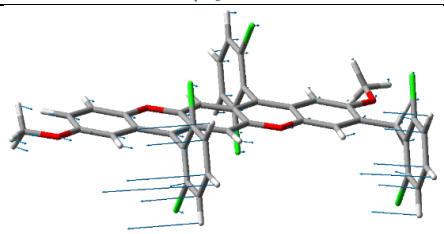
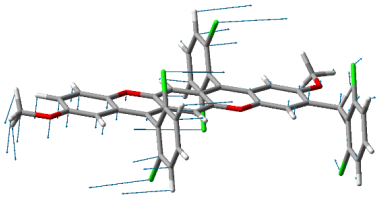
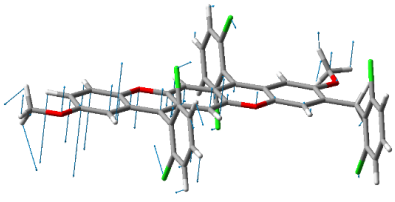
1 2

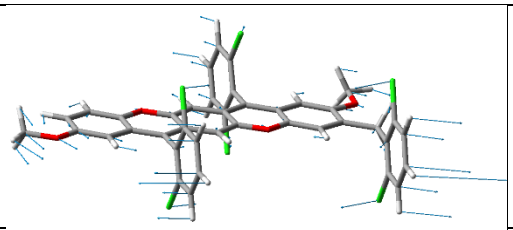
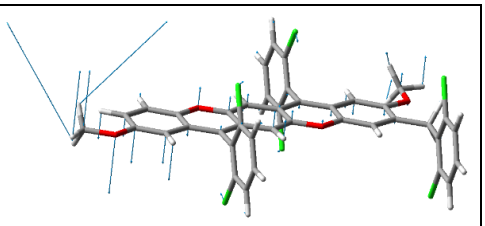
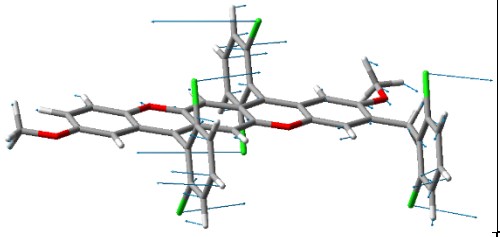
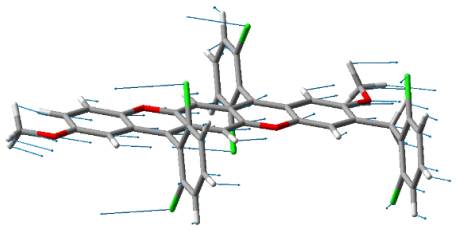
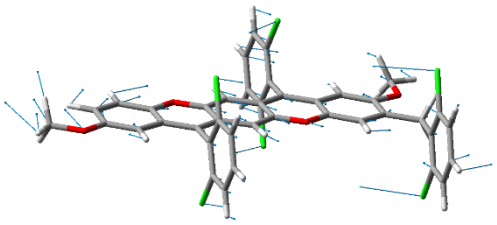
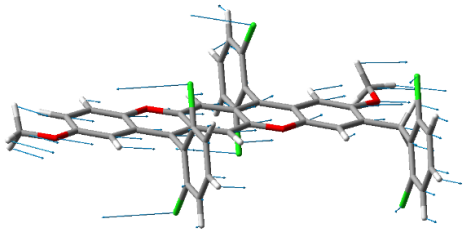
C	-0.99600000	3.57100000	2.73500000
C	-0.99700000	3.57100000	-2.73500000
C	-5.77600000	-2.28300000	-2.74800000
C	-5.77700000	-2.28100000	2.74900000
C	3.78700000	-2.22000000	2.73500000
C	3.78700000	-2.21900000	-2.73600000
O	-1.02300000	-0.61300000	0.00000000
O	3.81400000	1.97100000	0.00000000
O	-5.91900000	1.85600000	-0.00100000
O	8.62900000	-0.70500000	0.00000000
C	-2.19900000	0.06600000	0.00000000
C	-3.36400000	-0.70300000	0.00000000
H	-3.27300000	-1.78300000	0.00000000
C	-4.60600000	-0.08900000	0.00000000
C	-4.66500000	1.34500000	0.00000000
C	-3.51000000	2.10700000	0.00000000
H	-3.55800000	3.18700000	0.00000000
C	-2.23500000	1.48200000	0.00000000
C	-1.00300000	2.19500000	0.00000000
C	0.20900000	1.47700000	0.00000000
C	0.16700000	0.04000000	0.00000000
C	1.30400000	-0.73500000	0.00000000
H	1.20900000	-1.81400000	0.00000000
C	2.58400000	-0.12300000	0.00000000
C	2.62600000	1.31700000	0.00000000
C	1.48800000	2.09000000	0.00000000
H	1.58200000	3.16900000	0.00000000
C	4.99500000	1.29100000	0.00000000
C	6.16200000	2.05000000	0.00100000
H	6.09500000	3.13200000	0.00100000
C	7.39600000	1.41000000	0.00100000
H	8.29600000	2.01100000	0.00100000
C	7.46500000	-0.00500000	0.00000000
C	6.29600000	-0.75700000	0.00000000
H	6.36700000	-1.83800000	0.00000000
C	5.03100000	-0.12900000	0.00000000
C	3.79300000	-0.84300000	0.00000000
C	3.78600000	-2.33500000	0.00000000
C	3.78500000	-3.07200000	-1.19800000
C	3.78400000	-4.46500000	-1.21200000

H	3.78300000	-4.99700000	-2.15700000
C	3.78300000	-5.15700000	-0.00100000
H	3.78200000	-6.24200000	-0.00100000
C	3.78400000	-4.46600000	1.21100000
H	3.78300000	-4.99800000	2.15500000
C	3.78500000	-3.07200000	1.19700000
C	-0.99600000	3.68700000	0.00000000
C	-0.99300000	4.42400000	1.19800000
C	-0.98800000	5.81800000	1.21200000
H	-0.98500000	6.34900000	2.15600000
C	-0.98500000	6.50900000	0.00000000
H	-0.98000000	7.59400000	0.00000000
C	-0.98800000	5.81800000	-1.21200000
H	-0.98500000	6.35000000	-2.15600000
C	-0.99300000	4.42400000	-1.19800000
C	-5.91300000	-0.85600000	0.00000000
H	-6.49400000	-0.53600000	-0.87000000
H	-6.49400000	-0.53600000	0.86900000
C	-5.79200000	-2.36200000	0.00000000
C	-5.74100000	-3.11100000	-1.19000000
C	-5.66200000	-4.50300000	-1.20800000
H	-5.62900000	-5.03200000	-2.15400000
C	-5.62400000	-5.19700000	0.00100000
H	-5.56400000	-6.28000000	0.00100000
C	-5.66200000	-4.50300000	1.20900000
H	-5.63000000	-5.03100000	2.15500000
C	-5.74200000	-3.11100000	1.19100000
C	-6.08900000	3.28000000	0.00000000
H	-5.64600000	3.72400000	0.89700000
H	-7.16600000	3.44500000	0.00000000
H	-5.64700000	3.72400000	-0.89800000
C	9.87400000	0.00800000	0.00100000
H	9.97300000	0.62700000	-0.89600000
H	10.64700000	-0.76000000	0.00100000
H	9.97300000	0.62600000	0.89900000

Dipole: 7.5141 Debyes
Energy: -4638.81207741 Hartrees

Table S4. Low frequency (< 100 cm^{-1}) molecular vibrations present in an oxygen-embedded quinoidal pentacene. Displacement vectors shown scaled by 1.

Frequency (cm^{-1})	Vector Displacement	Frequency (cm^{-1})	Vector Displacement
7.07		23.84	
12.13		29.49	
14.89		42.94	
18.30		43.31	
20.09		44.24	
20.45		53.29	

61.90		75.61	
73.66		84.83	
75.45		89.05	

V. Calculated Absorption and Emission Transitions of DC

A. D3-B3LYP

Table S5. 30 CIS transitions of **DC** at the D3-B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.1626	573.30	0.3136	158 → 160 159 → 160	-0.21202 0.66084
2	2.4151	513.37	0.8713	158 → 160 159 → 160 159 → 162	0.6531 0.2068 0.1325
3	2.5792	480.72	0.0091	157 → 160 159 → 161	0.63362 -0.28337
4	2.8362	437.15	0.0238	154 → 160 156 → 160 157 → 160 158 → 161 159 → 161	-0.12354 0.21806 0.20699 -0.31570 0.52464
5	2.9001	427.51	0.0036	154 → 160 156 → 160 157 → 160 158 → 161	0.23594 0.63048 -0.10002 0.12280
6	2.9309	423.02	0.0168	153 → 160 155 → 160	0.30978 0.63129
7	2.9856	415.28	0.0469	153 → 160 155 → 160 159 → 162	0.60369 -0.28339 0.18986
8	2.9866	415.13	0.0111	150 → 160 154 → 160 156 → 160 157 → 160 158 → 161	-0.10640 0.63556 -0.15276 0.10122 -0.18535
9	3.1731	390.73	0.0303	152 → 160 158 → 161 159 → 161	0.24925 0.55129 0.29131
10	3.3354	371.73	0.0158	151 → 160 152 → 161 156 → 161 159 → 162	0.63275 -0.10460 0.14093 -0.22609
11	3.3488	370.24	0.2339	156 → 161 157 → 161	0.16217 0.66198

12	3.3689	368.03	0.0252	150 → 160 151 → 161 152 → 160 153 → 161 156 → 160 159 → 161	-0.30128 -0.11726 0.53905 -0.15774 0.10268 -0.13759
13	3.4936	354.89	1.4691	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.18144 0.14286 -0.14713 0.18895 -0.13451 0.56896
14	3.6016	344.25	0.0005	150 → 160 152 → 160 157 → 162	0.56149 0.26742 -0.26194
15	3.6038	344.03	0.0853	149 → 160 156 → 161	0.61963 0.26707
16	3.6822	336.71	0.0005	153 → 161 155 → 161 157 → 162	0.16587 0.67567 -0.10377
17	3.6854	336.42	0.0418	149 → 160 154 → 161 156 → 161	-0.13056 0.53287 0.41610
18	3.7380	331.68	0.2456	149 → 160 154 → 161 156 → 161 158 → 162 159 → 163	-0.13485 -0.33678 0.23814 0.49934 -0.13682
19	3.7470	330.89	0.0256	152 → 160 153 → 161 155 → 161 157 → 162	0.14212 0.62099 -0.11765 0.22737
20	3.8707	320.31	0.2198	150 → 161 151 → 160 152 → 161 153 → 162 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	-0.10145 0.15178 -0.13777 -0.11575 0.27216 -0.31463 0.14326 0.40372 0.17808
21	3.9886	310.85	0.0025	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.19723 -0.18887 0.13392 0.17058 0.56262
22	4.0921	302.98	0.0032	150 → 161 151 → 160 152 → 161 159 → 163	-0.24932 0.15333 0.58454 -0.20761

23	4.1432	299.25	0.0002	151 → 161 152 → 160	0.67097 0.10522
24	4.2204	293.77	0.0344	148 → 160 150 → 161 152 → 161 159 → 163	0.35495 -0.11535 0.17611 0.53638
25	4.2742	290.07	0.0170	149 → 161 156 → 162	0.65225 0.13084
26	4.2926	288.83	0.1104	148 → 160 150 → 161 152 → 161 159 → 163	0.38168 0.50633 0.17874 -0.15349
27	4.3417	285.57	0.0514	148 → 160 150 → 161 153 → 162 155 → 162	-0.20380 0.23132 0.30607 0.51690
28	4.3505	284.99	0.0006	154 → 162 156 → 162	0.51079 0.47393
29	4.3900	282.42	0.0884	148 → 160 150 → 161 152 → 161 153 → 162 155 → 162 158 → 163 159 → 163	0.20668 -0.15816 -0.14325 0.32554 0.11758 0.47701 -0.18953
30	4.4114	281.05	0.0043	149 → 161 152 → 162 154 → 162 156 → 162 157 → 163	0.17540 -0.12299 0.43642 -0.39795 -0.17246

Table S6. 30 D3-B3LYP TDDFT singlet transitions of **DC** at the D3-B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.0684	599.42	0.2724	158 → 160 159 → 160	-0.16394 0.68471
2	2.3512	527.33	0.6858	158 → 160 159 → 160 159 → 162	0.67661 0.16178 0.10737
3	2.5523	485.78	0.0121	157 → 160 159 → 161	0.66814 -0.20123
4	2.7671	448.06	0.0311	157 → 160 158 → 161 159 → 161	0.19402 -0.27042 0.60738
5	2.8730	431.55	0.0006	156 → 160	0.68744

6	2.9231	424.16	0.0154	153 → 160 155 → 160	0.28485 0.64325
7	2.9542	419.69	0.0348	153 → 160 155 → 160 159 → 162	0.61962 -0.26641 0.17093
8	2.9606	418.78	0.0052	154 → 160	0.69162
9	3.0981	400.20	0.0208	158 → 161 159 → 161	0.62947 0.25289
10	3.3038	375.28	0.0021	151 → 160 152 → 161 156 → 161 159 → 162	0.63423 -0.10809 0.14257 -0.20282
11	3.3054	375.10	0.2986	156 → 161 157 → 161	0.10946 0.68028
12	3.3182	373.65	0.011	150 → 160 151 → 161 152 → 160 153 → 161	-0.27483 -0.12638 0.60032 -0.12575
13	3.4028	364.36	0.9146	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.17609 0.14008 -0.14808 0.16978 -0.10963 0.59615
14	3.5425	349.99	0.0017	150 → 160 152 → 160 157 → 162	0.59697 0.27089 -0.19880
15	3.5653	347.75	0.1171	149 → 160 156 → 161 159 → 162	0.65893 0.16117 0.12383
16	3.6746	337.41	0.0781	149 → 160 151 → 160 154 → 161 156 → 161 158 → 162	-0.11254 -0.13560 0.30833 0.54398 0.24935
17	3.6777	337.12	0.0012	155 → 161	0.68946
18	3.7020	334.91	0.0944	154 → 161 158 → 162	0.52707 -0.44366
19	3.7199	333.30	0.0154	152 → 160 153 → 161 157 → 162	0.14196 0.65620 0.18698
20	3.7911	327.04	0.1694	151 → 160 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	0.15235 0.33251 -0.32019 0.12502 0.43688 0.15672

21	3.9358	315.02	0.0011	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.14927 -0.18433 0.12523 0.11187 0.62083
22	4.0716	304.51	0.0014	150 → 161 151 → 160 152 → 161 159 → 163	-0.17330 0.14386 0.58448 -0.27030
23	4.1243	300.62	0.0006	150 → 160 151 → 161 152 → 160	-0.11213 0.67199 0.10255
24	4.1636	297.78	0.0411	148 → 160 150 → 161 152 → 161 159 → 163	0.22507 -0.24004 0.21663 0.56365
25	4.2431	292.20	0.0122	149 → 161 156 → 162	0.65995 0.13726
26	4.2636	290.79	0.0357	148 → 160 150 → 161 152 → 161	0.38165 0.53247 0.21793
27	4.2943	288.72	0.2119	148 → 160 150 → 161 153 → 162 155 → 162 158 → 162 158 → 163 159 → 163	0.47638 -0.29527 -0.20615 -0.11972 -0.11859 0.11104 -0.23635
28	4.3393	285.72	0.0024	149 → 161 154 → 162 156 → 162	-0.10464 0.28046 0.61112
29	4.3587	284.45	0.0573	148 → 160 153 → 162 155 → 162 158 → 163	0.11554 0.27511 0.60168 0.15815
30	4.3676	283.87	0.084	153 → 162 155 → 162 158 → 163	0.37008 -0.29607 0.48916

Table S7. 30 D3-B3LYP TDA transitions of **DC** at the D3-B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.1626	573.30	0.3136	158 → 160 159 → 160	-0.21202 0.66084
2	2.4151	513.37	0.8713	158 → 160 159 → 160	0.65319 0.20680

				159 → 162	0.13252
3	2.5792	480.72	0.0091	157 → 160 159 → 161	0.63362 -0.28337
4	2.8362	437.15	0.0238	154 → 160 156 → 160 157 → 160 158 → 161 159 → 161	-0.12354 0.21806 0.20699 -0.31570 0.52464
5	2.9001	427.51	0.0036	154 → 160 156 → 160 157 → 160 158 → 161	0.23594 0.63048 -0.10002 0.12280
6	2.9309	423.02	0.0168	153 → 160 155 → 160	0.30978 0.63129
7	2.9856	415.28	0.0469	153 → 160 155 → 160 159 → 162	0.60369 -0.28339 0.18986
8	2.9866	415.13	0.0111	150 → 160 154 → 160 156 → 160 157 → 160 158 → 161	-0.10640 0.63556 -0.15276 0.10122 -0.18535
9	3.1731	390.73	0.0303	152 → 160 158 → 161 159 → 161	0.24925 0.55129 0.29131
10	3.3354	371.73	0.0158	151 → 160 152 → 161 156 → 161 159 → 162	0.63275 -0.10460 0.14093 -0.22609
11	3.3488	370.24	0.2339	156 → 161 157 → 161	0.16217 0.66198
12	3.3689	368.03	0.0252	150 → 160 151 → 161 152 → 160 153 → 161 156 → 160 159 → 161	-0.30128 -0.11726 0.53905 -0.15774 0.10268 -0.13759
13	3.4936	354.89	1.4691	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.18144 0.14286 -0.14713 0.18895 -0.13451 0.56896
14	3.6016	344.25	0.0005	150 → 160 152 → 160 157 → 162	0.56149 0.26742 -0.26194
15	3.6038	344.03	0.0853	149 → 160 156 → 161	0.61963 0.26707

16	3.6822	336.71	0.0005	153 → 161 155 → 161 157 → 162	0.16587 0.67567 -0.10377
17	3.6854	336.42	0.0418	149 → 160 154 → 161 156 → 161	-0.13056 0.53287 0.41610
18	3.7380	331.68	0.2456	149 → 160 154 → 161 156 → 161 158 → 162 159 → 163	-0.13485 -0.33678 0.23814 0.49934 -0.13682
19	3.7470	330.89	0.0256	152 → 160 153 → 161 155 → 161 157 → 162	0.14212 0.62099 -0.11765 0.22737
20	3.8707	320.31	0.2198	150 → 161 151 → 160 152 → 161 153 → 162 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	-0.10145 0.15178 -0.13777 -0.11575 0.27216 -0.31462 0.14326 0.40372 0.17808
21	3.9886	310.85	0.0025	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.19723 -0.18887 0.13392 0.17058 0.56262
22	4.0921	302.98	0.0032	150 → 161 151 → 160 152 → 161 159 → 163	-0.24932 0.15333 0.58454 -0.20761
23	4.1432	299.25	0.0002	151 → 161 152 → 160	0.67097 0.10522
24	4.2204	293.77	0.0344	148 → 160 150 → 161 152 → 161 159 → 163	0.35495 -0.11535 0.17611 0.53638
25	4.2742	290.07	0.0170	149 → 161 156 → 162	0.65225 0.13084
26	4.2926	288.83	0.1104	148 → 160 150 → 161 152 → 161 159 → 163	0.38168 0.50633 0.17874 -0.15349
27	4.3417	285.57	0.0514	148 → 160 150 → 161 153 → 162 155 → 162	-0.20380 0.23132 0.30607 0.51690

28	4.3505	284.99	0.0006	154 → 162 156 → 162	0.51079 0.47393
29	4.3900	282.42	0.0884	148 → 160 150 → 161 152 → 161 153 → 162 155 → 162 158 → 163 159 → 163	0.20668 -0.15815 -0.14325 0.32554 0.11758 0.47701 -0.18953
30	4.4114	281.05	0.0043	149 → 161 152 → 162 154 → 162 156 → 162 157 → 163	0.17540 -0.12299 0.43642 -0.39795 -0.17246

Table S8. 10 D3-B3LYP TDDFT triplet transitions of **DC** at the D3-B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	1.4377	862.39	0.0000	157A → 161A 159A → 160A 157B → 161B 159B → 160B	0.15442 0.67840 -0.15442 -0.67840
2	1.8593	666.84	0.0000	156A → 160A 157A → 160A 158A → 161A 159A → 161A 156B → 160B 157B → 160B 158B → 161B 159B → 161B	-0.13679 0.49019 0.12411 0.44784 0.13679 -0.49019 -0.12411 -0.44784
3	1.8937	654.72	0.0000	158A → 160A 158B → 160B	-0.67689 0.67689
4	2.4538	505.28	0.0000	152A → 160A 154A → 160A 156A → 160A 157A → 160A 158A → 161A 159A → 161A 152B → 160B 154B → 160B 156B → 160B 157B → 160B 158B → 161B 159B → 161B	-0.13977 -0.12307 0.26642 0.40190 0.23425 -0.39691 0.13977 0.12307 -0.26642 -0.40190 -0.23425 0.39691

5	2.5495	486.30	0.0000	149A → 160A 153A → 160A 154A → 161A 155A → 160A 156A → 161A 157A → 161A 159A → 160A 159A → 162A 149B → 160B 153B → 160B 154B → 161B 155B → 160B 156B → 161B 157B → 161B 159B → 160B 159B → 162B	0.23056 -0.44124 0.10831 0.25964 -0.12995 0.29877 -0.11682 -0.13096 -0.23056 0.44124 -0.10831 -0.25964 0.12995 -0.29877 0.11682 0.13096
6	2.5759	481.32	0.0000	150A → 160A 152A → 160A 153A → 161A 154A → 160A 156A → 160A 157A → 160A 158A → 161A 159A → 161A 150B → 160B 152B → 160B 153B → 161B 154B → 160B 156B → 160B 157B → 160B 158B → 161B 159B → 161B	0.18283 0.16131 -0.14508 0.16644 -0.25750 0.26285 -0.39004 -0.28486 -0.18283 -0.16131 0.14508 -0.16644 0.25750 -0.26285 0.39004 0.28486
7	2.7805	445.91	0.0000	150A → 161A 151A → 160A 155A → 160A 157A → 161A 158A → 162A 159A → 162A 150B → 161B 151B → 160B 155B → 160B 157B → 161B 158B → 162B 159B → 162B	-0.16301 -0.31976 -0.40976 0.20437 -0.12282 -0.32002 0.16301 0.31976 0.40976 -0.20437 0.12282 0.32002

8	2.7897	444.43	0.0000	150A → 160A 151A → 161A 154A → 160A 156A → 160A 158A → 161A 159A → 161A 150B → 160B 151B → 161B 154B → 160B 156B → 160B 158B → 161B 159B → 161B	0.15573 0.10818 -0.17933 0.46344 -0.37133 0.20889 -0.15573 -0.10818 0.17933 -0.46344 0.37133 -0.20889
9	2.8255	438.81	0.0000	150A → 160A 151A → 161A 152A → 160A 154A → 160A 156A → 160A 158A → 161A 150B → 160B 151B → 161B 152B → 160B 154B → 160B 156B → 160B 158B → 161B	0.28965 0.14415 -0.11995 0.51064 0.23641 0.14945 -0.28965 -0.14415 0.11995 -0.51064 -0.23641 -0.14945
10	2.8403	436.51	0.0000	151A → 160A 153A → 160A 155A → 160A 157A → 161A 158A → 162A 159A → 162A 151B → 160B 153B → 160B 155B → 160B 157B → 161B 158B → 162B 159B → 162B	-0.13061 -0.39860 -0.31578 -0.14602 0.20137 0.31645 0.13061 0.39860 0.31578 0.14602 -0.20137 -0.31645

Table S9. 30 D3-B3LYP TDDFT singlet transitions of **DC** at the D3-BLYP TDDFT S_2 optimized geometry (excited state 2 in Table S6).

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	1.9595	632.75	0.1821	158 → 160 159 → 160	-0.22319 0.66808
2	2.1852	567.39	0.7646	158 → 160 159 → 160 159 → 162	0.65983 0.22088 0.10967

3	2.4370	508.76	0.0169	157 → 160 159 → 161	0.68065 -0.15710
4	2.7170	456.33	0.0240	157 → 160 158 → 161 159 → 161	0.14725 -0.32974 0.59367
5	2.7918	444.10	0.0011	156 → 160	0.68952
6	2.8307	438.00	0.0150	153 → 160 155 → 160	-0.27483 0.64713
7	2.8663	432.56	0.0379	153 → 160 155 → 160 159 → 162	0.62572 0.25218 -0.17717
8	2.8739	431.41	0.0046	154 → 160	0.69300
9	3.0037	412.77	0.0254	152 → 160 158 → 161 159 → 161	-0.12064 0.60224 0.30940
10	3.2230	384.68	0.1047	151 → 160 156 → 161 159 → 162	0.60072 -0.11717 0.31197
11	3.2653	379.71	0.0120	150 → 160 151 → 161 152 → 160 153 → 161	0.30425 -0.11749 0.59031 -0.10983
12	3.2669	379.51	0.0429	156 → 161 157 → 161 159 → 162	0.10694 0.66545 0.14247
13	3.2837	377.57	1.1703	149 → 160 151 → 160 153 → 160 155 → 160 156 → 161 157 → 161 158 → 160 158 → 162 159 → 162	-0.11592 -0.27541 0.15537 0.10033 0.11962 -0.15805 -0.10727 -0.11626 0.54864
14	3.4626	358.06	0.0010	150 → 160 152 → 160 157 → 162	0.58133 -0.28349 -0.22607
15	3.5275	351.48	0.0421	156 → 161 158 → 162	0.15430 0.65484
16	3.5368	350.55	0.0867	149 → 160	0.68011
17	3.6622	338.55	0.0050	155 → 161 157 → 162	0.64516 -0.24804
18	3.6776	337.13	0.0324	151 → 160 154 → 161 156 → 161	0.10720 0.45893 0.51418

19	3.7011	334.99	0.0117	152 → 160 153 → 161 155 → 161 157 → 162	0.13398 0.60779 -0.17449 -0.25974
20	3.7583	329.89	0.1380	151 → 160 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	-0.15205 0.51639 -0.38647 0.10882 0.13472 0.11540
21	3.8271	323.97	0.0062	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.14825 0.31735 0.21492 0.11545 0.54262
22	4.0731	304.40	0.0006	148 → 160 150 → 161 151 → 160 152 → 161 159 → 163	0.23008 0.18595 0.11888 0.52125 0.30083
23	4.1106	301.62	0.0010	151 → 161 152 → 160	0.66614 0.10177
24	4.1323	300.04	0.0307	148 → 160 150 → 161 152 → 161 153 → 162 159 → 163	0.43341 -0.16022 -0.32983 -0.11237 0.38836
25	4.2015	295.10	0.1371	148 → 160 150 → 161 153 → 162 155 → 162 158 → 163 159 → 163	0.40986 0.23861 0.13963 -0.21944 0.15679 -0.38684
26	4.2313	293.02	0.0140	149 → 161 151 → 161 156 → 162 159 → 164	0.21925 -0.11806 0.60813 0.12943
27	4.2386	292.51	0.0615	150 → 161 153 → 162 155 → 162 158 → 163	-0.38092 0.48662 -0.13428 -0.25896
28	4.2525	291.56	0.1753	148 → 160 155 → 162 158 → 163 159 → 163	0.17740 0.63583 -0.11138 -0.16598

29	4.2533	291.50	0.0059	149 → 161 154 → 162 159 → 164	-0.27314 0.61961 -0.10402
30	4.2779	289.83	0.1545	150 → 161 152 → 161 153 → 162 158 → 163 159 → 163	-0.42109 0.24422 -0.12525 0.45475 -0.12053

B. B3LYP

Table S10. 30 CIS transitions of **DC** at the B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.1732	570.52	0.3439	158 → 160 159 → 160	-0.20963 0.66134
2	2.4202	512.30	0.8522	158 → 160 159 → 160 159 → 162	0.65357 0.20439 0.13479
3	2.5862	479.41	0.0092	157 → 160 159 → 161	0.63536 -0.27825
4	2.8515	434.80	0.0218	154 → 160 156 → 160 157 → 160 158 → 161 159 → 161	-0.13376 0.27779 0.18665 -0.30160 0.51041
5	2.8964	428.06	0.0051	154 → 160 156 → 160 157 → 160 158 → 161 159 → 161	0.24533 0.61175 -0.11307 0.14555 -0.12368
6	2.9235	424.10	0.0158	153 → 160 155 → 160	0.25268 0.65623
7	2.9836	415.55	0.0455	153 → 160 155 → 160 159 → 162	0.62760 -0.22790 0.18895
8	2.9851	415.35	0.0136	150 → 160 154 → 160 156 → 160 157 → 160 158 → 161	-0.10940 0.62763 -0.13961 0.11317 -0.20047
9	3.1757	390.41	0.0285	152 → 160 158 → 161 159 → 161	0.24970 0.54958 0.29528
10	3.3287	372.47	0.0179	151 → 160 152 → 161 156 → 161 159 → 162	0.63423 -0.10625 0.13754 -0.22482
11	3.3573	369.30	0.2341	154 → 161 156 → 161 157 → 161	-0.10691 0.15479 0.66210
12	3.3637	368.60	0.0272	150 → 160 151 → 161 152 → 160 153 → 161 159 → 161	-0.29524 -0.11867 0.54114 -0.14988 -0.14610

13	3.4881	355.45	1.4143	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.19723 0.14389 -0.15066 0.18354 -0.13511 0.56526
14	3.5984	344.55	0.0876	149 → 160 150 → 160 156 → 161	0.57039 -0.21210 0.24903
15	3.5984	344.55	0.0154	149 → 160 150 → 160 152 → 160 156 → 161 157 → 162	0.23141 0.52281 0.24026 0.10107 -0.24578
16	3.6767	337.21	0.0005	153 → 161 155 → 161	0.12987 0.68444
17	3.6805	336.86	0.0457	149 → 160 154 → 161 156 → 161	-0.12918 0.51174 0.44311
18	3.7412	331.40	0.2889	149 → 160 154 → 161 156 → 161 158 → 162 159 → 163	-0.13021 -0.33970 0.21765 0.50779 -0.13594
19	3.7446	331.10	0.0246	152 → 160 153 → 161 157 → 162	0.13872 0.62742 0.22920
20	3.8669	320.63	0.2194	150 → 161 151 → 160 152 → 161 153 → 162 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	-0.10093 0.14951 -0.13459 -0.12213 0.29653 -0.30164 0.14902 0.39407 0.18172
21	3.9835	311.25	0.0027	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.19757 -0.19956 0.12052 0.16831 0.56120
22	4.0892	303.20	0.0028	150 → 161 151 → 160 152 → 161 159 → 163	-0.24790 0.15413 0.59242 -0.18791
23	4.1384	299.59	0.0003	151 → 161 152 → 160	0.67174 0.10770
24	4.2265	293.35	0.0198	148 → 160 152 → 161 159 → 163	0.40057 0.15979 0.51605

25	4.2674	290.54	0.0184	149 → 161 156 → 162	0.64838 0.14386
26	4.2905	288.97	0.1159	148 → 160 150 → 161 152 → 161 159 → 163	0.35400 0.51416 0.17165 -0.18228
27	4.3278	286.49	0.0212	148 → 160 150 → 161 153 → 162 155 → 162	-0.14675 0.20329 0.28712 0.57368
28	4.3323	286.18	0.0004	154 → 162 156 → 162	0.48768 0.49810
29	4.3974	281.95	0.1337	148 → 160 150 → 161 151 → 162 152 → 161 153 → 162 155 → 162 158 → 163 159 → 163	0.29375 -0.22726 -0.10692 -0.16239 0.25797 0.14098 0.33578 -0.27160
30	4.4029	281.60	0.0036	149 → 161 152 → 162 154 → 162 156 → 162 157 → 162 157 → 163	0.18349 -0.12775 0.45782 -0.37915 0.10237 -0.15520

Table S11. 30 B3LYP TDDFT transitions of **DC** at the B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.0776	596.78	0.2974	158 → 160 159 → 160	-0.16256 0.68495
2	2.3575	525.92	0.6691	158 → 160 159 → 160 159 → 162	0.67662 0.16016 0.10927
3	2.5592	484.46	0.0124	157 → 160 159 → 161	0.66930 -0.19665
4	2.7826	445.56	0.0328	152 → 160 157 → 160 158 → 161 159 → 161	0.10046 0.18935 -0.27228 0.60516
5	2.8698	432.03	0.0004	156 → 160 159 → 161	0.68792 0.10548
6	2.9160	425.19	0.0148	153 → 160 155 → 160	0.21839 0.66868

7	2.9537	419.76	0.0334	153 → 160 155 → 160 159 → 162	0.64461 -0.20069 0.16967
8	2.9567	419.34	0.0058	154 → 160	0.69065
9	3.1029	399.57	0.0194	158 → 161 159 → 161	0.62852 0.25539
10	3.2967	376.08	0.0072	151 → 160 152 → 161 156 → 161 159 → 162	0.63661 -0.10940 0.14477 -0.20829
11	3.3120	374.34	0.0117	150 → 160 151 → 161 152 → 160 153 → 161	-0.26843 -0.12790 0.60357 -0.11864
12	3.3135	374.18	0.3241	157 → 161	0.68238
13	3.3977	364.91	0.8521	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.18599 0.14088 -0.15084 0.16796 -0.11041 0.58998
14	3.5391	350.32	0.0020	150 → 160 152 → 160 157 → 162	0.59953 0.26408 -0.20068
15	3.5588	348.39	0.1285	149 → 160 156 → 161 159 → 162	0.65680 0.15979 0.13374
16	3.6708	337.76	0.0713	149 → 160 151 → 160 154 → 161 156 → 161 158 → 162	-0.10667 -0.12768 0.32690 0.55573 0.20721
17	3.6727	337.58	0.0010	155 → 161	0.69299
18	3.7032	334.80	0.1283	154 → 161 158 → 162	0.49102 -0.47710
19	3.7192	333.37	0.0149	152 → 160 153 → 161 157 → 162	0.13810 0.65619 0.19318
20	3.7876	327.35	0.1703	151 → 160 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	0.15079 0.36299 -0.30475 0.12906 0.42300 0.15931
21	3.9307	315.42	0.0012	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.14970 -0.19600 0.11285 0.10945 0.61919

22	4.0698	304.64	0.0009	150 → 161 151 → 160 152 → 161 159 → 163	-0.17931 0.14750 0.59880 -0.23275
23	4.1196	300.96	0.0007	150 → 160 151 → 161 152 → 160	-0.11117 0.67214 0.10554
24	4.1722	297.16	0.0264	148 → 160 150 → 161 152 → 161 159 → 163	0.26747 -0.24438 0.17747 0.55876
25	4.2357	292.71	0.0131	149 → 161 154 → 162 156 → 162	0.65655 -0.10367 0.14647
26	4.2602	291.03	0.0360	148 → 160 150 → 161 152 → 161	0.39979 0.52253 0.20971
27	4.2920	288.87	0.1948	148 → 160 150 → 161 153 → 162 155 → 162 158 → 162 159 → 163	0.42964 -0.29870 -0.23648 -0.18148 -0.12231 -0.26358
28	4.3228	286.82	0.0016	149 → 161 154 → 162 156 → 162	-0.10126 0.30379 0.61006
29	4.3419	285.55	0.0986	148 → 160 153 → 162 155 → 162 159 → 163	0.15168 0.11484 0.65271 -0.12353
30	4.3635	284.14	0.0022	149 → 161 154 → 162 156 → 162 157 → 163 159 → 164	0.17144 0.60006 -0.21341 -0.10706 -0.12603

C. CAM-B3LYP

Table S12. 30 CIS transitions of **DC** at the CAM-B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.1451	577.99	0.2868	158 → 160 159 → 160	-0.16013 0.68535
2	2.4164	513.10	0.6723	158 → 160 159 → 160 159 → 162	0.67772 0.15812 0.10437
3	2.6094	475.14	0.0135	157 → 160 159 → 161	0.67413 0.17802
4	2.8409	436.42	0.0309	152 → 160 157 → 160 158 → 161 159 → 161	-0.10171 -0.17206 -0.27387 0.60617
5	2.9232	424.14	0.0003	156 → 160 159 → 161	0.68393 -0.12647
6	2.9748	416.78	0.0176	153 → 160 155 → 160	0.27966 0.64551
7	3.0054	412.54	0.0426	153 → 160 155 → 160 159 → 162	0.62537 -0.26267 0.15739
8	3.0095	411.98	0.0054	154 → 160	0.69314
9	3.1603	392.32	0.0196	158 → 161 159 → 161	0.62992 0.25734
10	3.3536	369.70	0.0885	151 → 160 152 → 161 157 → 161	0.53950 0.10333 0.40819
11	3.3599	369.01	0.2085	151 →160 156 → 161 157 → 161 159 → 162	-0.35267 0.17751 0.54992 0.14214
12	3.3604	368.96	0.0110	150 → 160 151 → 161 152 → 160 153 → 161	-0.25965 0.12657 0.60809 0.12036
13	3.4752	356.77	0.8363	149 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.21892 -0.12641 -0.16812 -0.10483 0.59943
14	3.5964	344.75	0.0018	150 → 160 152 → 160 157 → 162	0.60409 0.25827 -0.19363
15	3.6102	343.42	0.1630	149 → 160 156 → 161 159 → 162	0.64287 -0.18352 0.16274
16	3.7252	332.83	0.0731	149 → 160 151 → 160	0.11567 0.13296

				154 → 161	0.39797
				156 → 161	0.52112
				158 → 162	-0.15466
17	3.7253	332.82	0.0012	155 → 161	0.69004
18	3.7609	329.66	0.1515	154 → 161	0.51180
				156 → 161	-0.20886
				158 → 162	0.39727
19	3.7657	329.24	0.0139	152 → 160	-0.13258
				153 → 161	0.66280
				157 → 162	-0.17224
20	3.8498	322.06	0.1722	151 → 160	0.13134
				154 → 161	-0.25218
				156 → 161	0.27360
				157 → 161	-0.12079
				158 → 162	0.51701
				159 → 162	0.15369
21	3.9947	310.37	0.0005	150 → 160	0.14695
				153 → 161	0.16662
				155 → 161	-0.12005
				156 → 162	0.11358
				157 → 162	0.62587
22	4.1157	301.25	0.0020	150 → 161	-0.17708
				151 → 160	-0.14922
				152 → 161	0.61219
				159 → 163	0.20099
23	4.1717	297.20	0.0009	150 → 160	0.11470
				151 → 161	0.67171
				152 → 160	-0.10274
24	4.2364	292.67	0.0192	148 → 160	0.27664
				150 → 161	0.24918
				152 → 161	-0.14268
				159 → 163	0.56348
25	4.2831	289.47	0.0118	149 → 161	0.66485
				156 → 162	-0.12662
26	4.3179	287.14	0.0421	148 → 160	-0.37424
				150 → 161	0.54351
				152 → 161	0.20655
27	4.3537	284.78	0.2081	148 → 160	0.46058
				150 → 161	0.26533
				153 → 162	-0.20982
				155 → 162	-0.13049
				158 → 162	-0.12439
				159 → 163	-0.29096
28	4.3967	281.99	0.0029	154 → 162	0.24939
				156 → 162	0.62437
29	4.4187	280.59	0.0801	148 → 160	0.12092
				153 → 162	0.19991
				155 → 162	0.64459
				159 → 163	-0.10857

30	4.4282	279.99	0.0020	149 → 161 154 → 162 156 → 162 159 → 164	-0.13228 0.63525 -0.17118 -0.10133

Table S13. 30 CAM-B3LYP TDDFT transitions of **DC** at the CAM-B3LYP ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.1451	577.99	0.2868	158 → 160 159 → 160	-0.16013 0.68535
2	2.4164	513.10	0.6723	158 → 160 159 → 160 159 → 162	0.67772 0.15812 0.10437
3	2.6094	475.14	0.0135	157 → 160 159 → 161	0.67413 0.17802
4	2.8409	436.42	0.0309	152 → 160 157 → 160 158 → 161 159 → 161	-0.10171 -0.17206 -0.27387 0.60617
5	2.9232	424.14	0.0003	156 → 160 159 → 161	0.68393 -0.12647
6	2.9748	416.78	0.0176	153 → 160 155 → 160	0.27966 0.64551
7	3.0054	412.54	0.0426	153 → 160 155 → 160 159 → 162	0.62537 -0.26267 0.15739
8	3.0095	411.98	0.0054	154 → 160	0.69314
9	3.1603	392.32	0.0196	158 → 161 159 → 161	0.62992 0.25734
10	3.3536	369.70	0.0885	151 → 160 152 → 161 157 → 161	0.53950 0.10333 0.40819
11	3.3599	369.01	0.2085	151 → 160 156 → 161 157 → 161 159 → 162	-0.35267 0.17751 0.54992 0.14214
12	3.3604	368.96	0.0110	150 → 160 151 → 161 152 → 160 153 → 161	-0.25965 0.12657 0.60809 0.12036
13	3.4752	356.77	0.8363	149 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.21892 -0.12641 -0.16812 -0.10483 0.59943
14	3.5964	344.75	0.0018	150 → 160 152 → 160 157 → 162	0.60409 0.25827 -0.19363

15	3.6102	343.42	0.1630	149 → 160 156 → 161 159 → 162	0.64287 -0.18352 0.16274
16	3.7252	332.83	0.0731	149 → 160 151 → 160 154 → 161 156 → 161 158 → 162	0.11567 0.13296 0.39797 0.52112 -0.15466
17	3.7253	332.82	0.0012	155 → 161	0.69004
18	3.7609	329.66	0.1515	154 → 161 156 → 161 158 → 162	0.51180 -0.20886 0.39727
19	3.7657	329.24	0.0139	152 → 160 153 → 161 157 → 162	-0.13258 0.66280 -0.17224
20	3.8498	322.06	0.1722	151 → 160 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	0.13134 -0.25218 0.27360 -0.12079 0.51701 0.15369
21	3.9947	310.37	0.0005	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.14695 0.16662 -0.12005 0.11358 0.62587
22	4.1157	301.25	0.0020	150 → 161 151 → 160 152 → 161 159 → 163	-0.17708 -0.14922 0.61219 0.20099
23	4.1717	297.20	0.0009	150 → 160 151 → 161 152 → 160	0.11470 0.67171 -0.10274
24	4.2364	292.67	0.0192	148 → 160 150 → 161 152 → 161 159 → 163	0.27664 0.24918 -0.14268 0.56348
25	4.2831	289.47	0.0118	149 → 161 156 → 162	0.66485 -0.12662
26	4.3179	287.14	0.0421	148 → 160 150 → 161 152 → 161	-0.37424 0.54351 0.20655
27	4.3537	284.78	0.2081	148 → 160 150 → 161 153 → 162 155 → 162 158 → 162 159 → 163	0.46058 0.26533 -0.20982 -0.13049 -0.12439 -0.29096
28	4.3967	281.99	0.0029	154 → 162 156 → 162	0.24939 0.62437

29	4.4187	280.59	0.0801	148 → 160 153 → 162 155 → 162 159 → 163	0.12092 0.19991 0.64459 -0.10857
30	4.4282	279.99	0.0020	149 → 161 154 → 162 156 → 162 159 → 164	-0.13228 0.63525 -0.17118 -0.10133

D. PBE0

Table S14. 30 CIS transitions of **DC** at the PBE0 ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.1850	567.43	0.3354	158 → 160 159 → 160	0.21050 0.66138
2	2.4362	508.92	0.8592	158 → 160 159 → 160 159 → 162	0.65381 -0.20556 -0.13193
3	2.6002	476.83	0.0088	157 → 160 159 → 161	0.63617 -0.27702
4	2.8645	432.82	0.0228	154 → 160 156 → 160 157 → 160 158 → 161 159 → 161	-0.12423 0.22795 0.19865 0.31072 0.52682
5	2.9319	422.89	0.0038	154 → 160 156 → 160 158 → 161	0.25948 0.61960 -0.12894
6	2.9613	418.69	0.0161	153 → 160 155 → 160	0.32140 0.62541
7	3.0136	411.41	0.0490	153 → 160 155 → 160 159 → 162	0.59832 -0.29401 -0.19305
8	3.0145	411.29	0.0121	150 → 160 154 → 160 156 → 160 157 → 160 158 → 161	-0.10581 0.62709 -0.17065 0.10434 0.19570
9	3.2030	387.08	0.0297	152 → 160 158 → 161 159 → 161	-0.24761 0.55031 -0.29207
10	3.3621	368.77	0.0292	151 → 160 156 → 161 159 → 162	0.63417 -0.15587 0.21307
11	3.3758	367.28	0.2125	156 → 161 157 → 161	0.14692 0.66224
12	3.3969	364.99	0.0249	150 → 160 151 → 161 152 → 160 153 → 161 156 → 160 159 → 161	-0.30654 0.11815 0.53911 0.14884 0.10759 -0.13871
13	3.5234	351.88	1.4400	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.19413 -0.14007 0.14397 0.18565 0.13322 0.56827

14	3.6292	341.63	0.0006	150 → 160 152 → 160 157 → 162	0.56068 0.27195 -0.25858
15	3.6331	341.26	0.1123	149 → 160 156 → 161 159 → 162	0.61982 0.25844 0.10168
16	3.7195	333.34	0.0005	153 → 161 155 → 161 157 → 162	0.16779 0.67445 0.10769
17	3.7235	332.98	0.0359	149 → 160 154 → 161 156 → 161	-0.11258 0.55401 0.39665
18	3.7729	328.62	0.2737	149 → 160 154 → 161 156 → 161 158 → 162 159 → 163	0.12447 0.31958 -0.26005 0.50116 0.13921
19	3.7783	328.15	0.0231	152 → 160 153 → 161 155 → 161 157 → 162	-0.13674 0.62318 -0.11674 -0.22907
20	3.9033	317.64	0.2219	151 → 160 152 → 161 153 → 162 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	0.14534 0.13997 -0.11284 -0.25515 0.32966 -0.14222 0.40474 -0.17853
21	4.0197	308.44	0.0027	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.19126 0.18902 -0.13934 0.17096 0.56496
22	4.1275	300.39	0.0040	150 → 161 151 → 160 152 → 161 159 → 163	-0.25323 -0.15007 0.57825 -0.21784
23	4.1761	296.89	0.0003	151 → 161 152 → 160	0.67339 -0.10451
24	4.2504	291.70	0.0332	148 → 160 150 → 161 152 → 161 159 → 163	0.34623 -0.12606 0.18605 0.53581
25	4.3069	287.87	0.0169	149 → 161 156 → 162	0.65129 0.13205
26	4.3274	286.51	0.1121	148 → 160 150 → 161 152 → 161 159 → 163	0.38227 0.50762 0.18522 -0.14339

27	4.3800	283.07	0.0663	148 → 160 150 → 161 153 → 162 155 → 162 158 → 163 159 → 163	0.23653 -0.24178 0.29576 0.48815 -0.10384 -0.11538
28	4.3932	282.22	0.0006	154 → 162 156 → 162	0.54159 0.44024
29	4.4255	280.16	0.0799	148 → 160 150 → 161 152 → 161 153 → 162 155 → 162 158 → 163 159 → 163	-0.19532 0.14374 0.13809 0.34859 0.15015 0.46901 0.17647
30	4.4471	278.80	0.0034	149 → 161 152 → 162 154 → 162 156 → 162 157 → 163 159 → 165	-0.18034 0.12150 -0.40093 0.42390 0.17768 0.11857

Table S15. 30 PBE0 TDDFT transitions of **DC** at the PBE0 ground state singlet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	
1	2.0898	593.29	0.2904	158 → 160 159 → 160	0.16276 0.68501
2	2.3733	522.42	0.6744	158 → 160 159 → 160 159 → 162	0.67691 -0.16064 -0.10701
3	2.5732	481.83	0.0117	157 → 160 159 → 161	0.66926 -0.19686
4	2.7962	443.40	0.0307	157 → 160 158 → 161 159 → 161	0.18896 0.26911 0.60975
5	2.9035	427.02	0.0008	156 → 160	0.68576
6	2.9534	419.80	0.0153	153 → 160 155 → 160	0.29302 0.63943
7	2.9833	415.60	0.0371	153 → 160 155 → 160 159 → 162	0.61658 -0.27367 -0.17310
8	2.9884	414.88	0.0057	154 → 160	0.69103
9	3.1281	396.36	0.0200	158 → 161 159 → 161	0.62915 -0.25235
10	3.3301	372.31	0.0488	151 → 160 156 → 161 157 → 161 159 → 162	0.60952 -0.17343 -0.17318 0.20259

11	3.3334	371.94	0.2401	151 → 160 157 → 161	0.19723 0.66383
12	3.3465	370.49	0.0106	150 → 160 151 → 161 152 → 160 153 → 161	-0.27977 0.12646 0.59989 0.11955
13	3.4322	361.23	0.9090	149 → 160 151 → 160 153 → 160 156 → 161 158 → 160 159 → 162	-0.18359 -0.13073 0.14505 0.16816 0.10909 0.59850
14	3.5696	347.34	0.0018	150 → 160 152 → 160 157 → 162	0.59573 0.27544 -0.19597
15	3.5934	345.03	0.1343	149 → 160 156 → 161 159 → 162	0.65791 0.15461 0.13313
16	3.7135	333.88	0.0822	149 → 160 151 → 160 154 → 161 156 → 161 158 → 162	-0.10232 0.13150 0.32094 0.53286 -0.26275
17	3.7147	333.76	0.0013	155 → 161 157 → 162	0.68872 0.10688
18	3.7372	331.76	0.1023	154 → 161 158 → 162	0.53336 0.43504
19	3.7536	330.31	0.0138	152 → 160 153 → 161 157 → 162	-0.13670 0.65817 -0.18716
20	3.8243	324.20	0.1735	151 → 160 154 → 161 156 → 161 157 → 161 158 → 162 159 → 162	0.14756 -0.31269 0.33876 -0.12455 0.43848 -0.15735
21	3.9676	312.49	0.0013	150 → 160 153 → 161 155 → 161 156 → 162 157 → 162	0.14439 0.18480 -0.13076 0.11240 0.62100
22	4.1062	301.95	0.0021	148 → 160 150 → 161 151 → 160 152 → 161 159 → 163	-0.10378 -0.17140 -0.13916 0.57444 -0.29111
23	4.1575	298.22	0.0007	150 → 160 151 → 161 152 → 160	0.11284 0.67332 -0.10183

24	4.1935	295.66	0.0404	148 → 160 150 → 161 152 → 161 159 → 163	0.21575 -0.24540 0.23692 0.55599
25	4.2759	289.96	0.0121	149 → 161 156 → 162	0.66022 0.13742
26	4.2977	288.49	0.0383	148 → 160 150 → 161 152 → 161	0.36707 0.53910 0.22527
27	4.3278	286.48	0.2036	148 → 160 150 → 161 153 → 162 155 → 162 158 → 162 158 → 163 159 → 163	0.49460 -0.28244 0.18690 0.10758 0.11845 -0.10936 -0.23300
28	4.3821	282.93	0.0023	149 → 161 154 → 162 156 → 162	-0.10818 0.27262 0.60675
29	4.3995	281.82	0.0427	153 → 162 155 → 162 158 → 163	0.35181 0.53064 0.25205
30	4.4045	281.50	0.0841	153 → 162 155 → 162 158 → 163	0.28239 -0.40538 0.46700

VI. Calculated Absorption and Emission Transitions of RC

A. D3-B3LYP

Table S16. 30 CIS transitions of **RC** at the D3-B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	1.0600	1169.67	0.5013	160A → 161A 0.95570 158B → 160B -0.17944 159B → 160B -0.13749	0.785
2	1.6405	755.78	0.0000	160A → 162A 0.97141	0.830
3	1.8784	660.04	0.1839	157A → 161A -0.14725 160A → 161A 0.10793 160A → 164A 0.10158 158B → 160B -0.14550 159B → 160B 0.94262	0.871
4	2.1254	583.34	0.0001	159A → 161A 0.70642 160A → 162A -0.13515 160A → 163A -0.17287 157B → 160B -0.44458 159B → 161B -0.44591	2.167
5	2.3155	535.46	0.6271	157A → 161A -0.14434 159A → 162A -0.11876 160A → 161A 0.16537 160A → 164A -0.10433 158B → 160B 0.91914 159B → 160B 0.10194 159B → 162B 0.12143	0.895
6	2.3456	528.57	0.0001	158A → 161A -0.11482 159A → 161A 0.28267 160A → 163A 0.89988 157B → 160B 0.16428 158B → 161B 0.13512	1.000
7	2.5918	478.38	0.0048	158A → 161A 0.78202 159A → 161A -0.20623 160A → 163A 0.29086 160A → 166A -0.10271 152B → 160B 0.11032 156B → 160B -0.15761 157B → 160B -0.28624 158B → 161B -0.30520	2.046
8	2.6554	466.91	0.0061	158A → 161A 0.33984 159A → 161A 0.11335 160A → 163A -0.14606 157B → 160B 0.75463 159B → 161B -0.46016	1.343

9	2.6836	462.01	0.0371	157A → 161A 0.34054 158A → 162A 0.11190 159A → 162A 0.14246 160A → 164A 0.75317 160A → 165A -0.18974 157B → 161B -0.23851 158B → 160B 0.16574 158B → 162B 0.17907 159B → 162B 0.21000	1.393
10	2.7457	451.56	0.0535	157A → 161A -0.30123 159A → 162A -0.11846 160A → 164A 0.50650 160A → 165A 0.57119 160A → 171A -0.12822 149B → 160B 0.13308 155B → 160B 0.34064 157B → 161B 0.25027 159B → 160B -0.12127 159B → 162B -0.13760	1.243
11	2.7787	446.19	0.0251	155A → 161A -0.11810 159A → 161A 0.47498 160A → 166A 0.33312 160A → 167A -0.19222 160A → 172A -0.13035 156B → 160B -0.26085 157B → 160B 0.13225 158B → 161B -0.30131 159B → 161B 0.61239	0.951
12	2.8161	440.27	0.0835	157A → 161A 0.29279 159A → 162A 0.10541 160A → 164A -0.22981 160A → 165A 0.75284 160A → 169A -0.11746 151B → 160B 0.12824 155B → 160B -0.21124 157B → 161B -0.26316 159B → 160B 0.12991 159B → 162B 0.26175	1.279
13	2.8216	439.41	0.0017	158A → 161A 0.12701 159A → 161A -0.17554 160A → 166A 0.88000 152B → 160B -0.12921 156B → 160B 0.13478 158B → 161B 0.15458 159B → 161B -0.14406	0.868

14	3.005	412.60	0.0984	159A → 162A 0.45193 159A → 163A 0.16748 160A → 164A -0.17314 160A → 168A -0.36835 160A → 171A -0.15033 155B → 160B 0.52097 159B → 162B 0.42087 159B → 163B -0.11141	1.773
15	3.0221	410.26	0.0036	158A → 161A 0.10946 151B → 161B 0.11560 152B → 160B 0.10494 156B → 160B 0.86778 157B → 160B 0.12840 157B → 162B 0.10561 158B → 161B -0.22869 159B → 161B 0.25212	1.052
16	3.0254	409.81	0.0879	156A → 161A -0.15196 157A → 161A -0.44259 158A → 162A -0.20101 159A → 162A 0.28434 160A → 164A 0.13848 160A → 168A 0.23172 155B → 160B -0.40384 157B → 161B 0.17571 158B → 162B -0.17434 159B → 160B -0.11597 159B → 162B 0.49053 159B → 163B -0.11847	2.085
17	3.0595	405.24	0.0001	158A → 161A -0.25433 160A → 167A 0.81485 160A → 170A -0.11661 152B → 160B 0.13261 153B → 160B -0.13755 156B → 160B -0.13010 157B → 160B 0.11865 158B → 161B -0.34738	0.847
18	3.1272	396.46	0.0003	157A → 161A 0.43677 160A → 168A 0.34302 160A → 169A 0.74630 160A → 171A -0.14753 151B → 160B -0.15339 157B → 161B 0.16671	0.920

19	3.1672	391.46	0.0058	151A → 161A -0.10979 156A → 161A -0.19918 158A → 162A -0.14365 160A → 165A -0.13818 150B → 161B 0.17638 151B → 160B 0.42027 154B → 160B 0.72197 155B → 160B 0.11734 156B → 161B 0.17646 158B → 162B -0.16868 159B → 162B -0.15353	1.239
20	3.1958	387.96	0.0022	149A → 161A -0.10370 152A → 161A -0.15574 155A → 161A -0.19819 160A → 166A 0.20955 160A → 167A 0.19928 160A → 172A -0.19194 150B → 160B 0.41114 151B → 161B 0.16512 152B → 160B 0.29519 153B → 160B 0.58255 155B → 161B 0.14145 158B → 161B 0.28713	1.185
21	3.2279	384.10	0.0043	158A → 162A -0.10006 159A → 162A 0.15169 160A → 168A 0.72402 160A → 169A -0.34246 149B → 160B -0.10140 154B → 160B -0.12657 155B → 160B 0.44431 157B → 161B -0.15700 158B → 162B -0.15780	0.984
22	3.2387	382.83	0.0096	157A → 162A -0.11263 158A → 161A 0.26474 159A → 161A 0.17138 160A → 167A 0.28403 160A → 170A 0.28901 152B → 160B 0.20189 153B → 160B -0.49740 158B → 161B 0.57389 159B → 161B 0.18942	0.900

23	3.2946	376.32	0.0206	156A → 161A 0.26340 157A → 161A -0.16644 158A → 162A 0.42086 160A → 168A 0.28719 160A → 169A -0.10790 149B → 160B 0.16777 151B → 160B -0.22036 154B → 160B 0.47211 155B → 160B -0.10237 158B → 162B 0.47400	1.827
24	3.2956	376.21	0.0002	160A → 167A 0.10335 160A → 170A 0.89138 160A → 172A 0.12815 152B → 160B -0.23212 153B → 160B 0.14266 158B → 161B -0.23757	0.876
25	3.3226	373.16	0.0103	156A → 161A 0.16906 158A → 162A -0.14421 160A → 168A -0.11356 160A → 169A 0.14660 160A → 171A 0.60292 149B → 160B -0.21848 150B → 161B -0.13597 151B → 160B -0.41441 154B → 160B 0.36530 155B → 160B 0.22847 157B → 161B -0.13550 158B → 162B -0.15588	1.099
26	3.3339	371.89	0.0103	152A → 161A 0.18808 154A → 161A 0.13601 155A → 161A 0.15557 158A → 161A 0.15175 159A → 161A 0.10384 160A → 166A -0.11304 160A → 167A 0.23373 160A → 172A 0.12551 150B → 160B -0.51423 151B → 161B -0.12313 152B → 160B -0.14332 153B → 160B 0.58106 155B → 161B -0.11540 158B → 161B 0.20089 159B → 161B 0.12844	1.062

27	3.3705	367.85	0.0092	156A → 161A 0.56166 157A → 161A 0.31186 158A → 162A -0.23360 159A → 162A -0.24189 160A → 168A -0.10791 160A → 169A -0.24298 160A → 171A -0.27000 154B → 160B 0.16197 155B → 160B -0.13495 157B → 161B 0.31726 158B → 162B -0.24810 159B → 162B 0.25596	1.430
28	3.4058	364.04	0.0412	150A → 161A -0.12939 156A → 161A 0.48286 158A → 162A 0.13668 160A → 169A 0.23522 160A → 171A 0.48054 149B → 160B 0.12271 150B → 161B 0.10825 151B → 160B 0.56446 154B → 160B -0.18746	1.082
29	3.4575	358.60	0.0068	155A → 161A 0.68221 157A → 162A 0.14870 160A → 172A -0.22005 150B → 160B 0.35140 151B → 161B 0.11168 152B → 160B -0.31975 155B → 161B -0.22417 156B → 160B -0.19816 157B → 160B 0.10062 157B → 162B 0.17198	1.851
30	3.4936	354.89	0.0034	152A → 161A -0.11545 154A → 161A -0.13084 155A → 161A 0.42111 157A → 162A 0.18455 160A → 167A -0.14728 160A → 170A 0.21278 160A → 172A -0.28096 150B → 160B -0.42526 152B → 160B 0.56419 157B → 162B -0.12159	0.977

Table S17. 30 D3-B3LYP TDDFT transitions of **RC** at the D3-B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$

1	0.9188	1349.45	0.3373	160A → 161A 0.97692 158B → 160B -0.13479 159B → 160B -0.13112	0.785
2	1.5875	780.98	0.0000	159A → 161A 0.14852 160A → 162A 0.96065 159B → 161B -0.13276	0.830
3	1.7900	692.66	0.1390	157A → 161A -0.15206 160A → 161A 0.12141 157B → 161B 0.11969 158B → 160B -0.12694 159B → 160B 0.94569	0.871
4	2.0444	606.46	0.0002	158A → 161A 0.10539 159A → 161A 0.68333 160A → 162A -0.22265 160A → 163A -0.15944 157B → 160B -0.43280 158B → 161B -0.10839 159B → 161B -0.44807	2.167
5	2.2315	555.61	0.4284	157A → 161A -0.13476 160A → 161A 0.14033 160A → 164A -0.12357 157B → 161B 0.11060 158B → 160B 0.92801	0.895
6	2.3048	537.95	0.0000	158A → 161A -0.13591 159A → 161A 0.28719 160A → 163A 0.89481 157B → 160B 0.17396 158B → 161B 0.12631	1.000
7	2.5577	484.75	0.0063	158A → 161A 0.75875 159A → 161A -0.29011 160A → 163A 0.32231 160A → 166A -0.10671 152B → 160B 0.10460 156B → 160B -0.12602 157B → 160B -0.28461 158B → 161B -0.27928	2.046
8	2.6093	475.17	0.0248	157A → 161A 0.44269 158A → 162A 0.17631 159A → 162A 0.18871 160A → 164A 0.54019 160A → 165A -0.19583 160A → 169A -0.10552 155B → 160B -0.19129 157B → 161B -0.32033 158B → 160B 0.17312 158B → 162B 0.20312 159B → 160B 0.13455 159B → 162B 0.25922	1.343

9	2.6239	472.51	0.0115	155A → 161A -0.10091 158A → 161A 0.37289 159A → 161A 0.21888 160A → 163A -0.16061 160A → 167A -0.10975 157B → 160B 0.78234 158B → 161B -0.14206 159B → 161B -0.27202	1.393
10	2.6928	460.43	0.0645	157A → 161A -0.23366 160A → 164A 0.71533 160A → 165A 0.37810 160A → 171A -0.13510 149B → 160B 0.13147 155B → 160B 0.32122 157B → 161B 0.20793 159B → 160B -0.12774 159B → 162B -0.10669	1.243
11	2.7115	457.25	0.0172	159A → 161A 0.47427 160A → 167A -0.10624 160A → 172A -0.10647 156B → 160B -0.27896 158B → 161B -0.28883 159B → 161B 0.74010	0.951
12	2.7841	445.33	0.0440	157A → 161A 0.19466 160A → 164A -0.24031 160A → 165A 0.85528 151B → 160B 0.11867 155B → 160B -0.11143 157B → 161B -0.17554 159B → 160B 0.10620 159B → 162B 0.21051	1.279
13	2.7873	444.81	0.0000	158A → 161A 0.12824 160A → 166A 0.91754 150B → 160B -0.12916 152B → 160B -0.12725	0.868
14	2.9477	420.61	0.0908	158A → 162A 0.12319 159A → 162A 0.40633 159A → 163A 0.19897 160A → 164A -0.17861 160A → 165A -0.12537 160A → 168A -0.30704 160A → 169A 0.12147 160A → 171A -0.15572 155B → 160B 0.49453 158B → 162B 0.12719 159B → 162B 0.42980 159B → 163B -0.16825	1.773

15	2.9843	415.46	0.0679	156A → 161A -0.13752 157A → 161A -0.41332 158A → 162A -0.18884 159A → 162A 0.25577 160A → 164A 0.16754 160A → 168A 0.23953 155B → 160B -0.42484 156B → 161B 0.10161 157B → 161B 0.12373 158B → 160B -0.10025 158B → 162B -0.17365 159B → 160B -0.11238 159B → 162B 0.51484 159B → 163B -0.11763	1.052
16	2.9892	414.77	0.0040	158A → 161A 0.14434 151B → 161B 0.12056 155B → 161B -0.11096 156B → 160B 0.86300 157B → 160B 0.11691 157B → 162B 0.10996 158B → 161B -0.10740 159B → 161B 0.29511	2.085
17	3.0224	410.21	0.0000	158A → 161A -0.27537 160A → 167A 0.77411 160A → 170A -0.14043 152B → 160B 0.15280 153B → 160B -0.13227 157B → 160B 0.13283 158B → 161B -0.39628	0.847
18	3.0949	400.61	0.0003	157A → 161A 0.38141 158A → 162A 0.11671 160A → 168A 0.38096 160A → 169A 0.68046 160A → 171A -0.12267 151B → 160B -0.28045 154B → 160B -0.13302 157B → 161B 0.15110	0.920

19	3.1207	397.30	0.0050	151A → 161A -0.12135 156A → 161A -0.19364 157A → 161A 0.19897 158A → 162A -0.19595 160A → 165A -0.14807 160A → 169A 0.24521 160A → 171A -0.10954 150B → 161B 0.18662 151B → 160B 0.41563 154B → 160B 0.58122 155B → 160B 0.14014 156B → 161B 0.17988 158B → 162B -0.23708	1.239
20	3.1462	394.08	0.0011	149A → 161A -0.10481 152A → 161A -0.17984 155A → 161A -0.18759 160A → 166A 0.26835 160A → 167A 0.21161 160A → 172A -0.19801 149B → 161B 0.11269 150B → 160B 0.44509 151B → 161B 0.18917 152B → 160B 0.32408 153B → 160B 0.45730 155B → 161B 0.15333 158B → 161B 0.30593	1.185
21	3.1753	390.47	0.0106	157A → 162A -0.10404 158A → 161A 0.30502 159A → 161A 0.17497 160A → 166A -0.11379 160A → 167A 0.40380 150B → 160B -0.12347 153B → 160B -0.33582 156B → 160B -0.11229 158B → 161B 0.65083 159B → 161B 0.16730	0.984
22	3.2056	386.77	0.0008	157A → 161A 0.18014 158A → 162A -0.20037 159A → 162A 0.14976 160A → 168A 0.59921 160A → 169A -0.32350 149B → 160B -0.13833 154B → 160B -0.24680 155B → 160B 0.47168 157B → 161B -0.10850 158B → 162B -0.24908 159B → 162B 0.11401	0.900

23	3.2441	382.18	0.0258	157A → 161A -0.26507 158A → 162A 0.38706 160A → 168A 0.49169 160A → 169A -0.20700 149B → 160B 0.16400 154B → 160B 0.40942 157B → 161B -0.12464 158B → 162B 0.41995	1.827
24	3.2819	377.78	0.0000	160A → 167A 0.17062 160A → 170A 0.91303 160A → 172A 0.12117 152B → 160B -0.17300 158B → 161B -0.17402	0.876
25	3.2955	376.23	0.0057	152A → 161A 0.14937 155A → 161A 0.11074 160A → 167A 0.21606 160A → 170A -0.11355 160A → 172A 0.12466 150B → 160B -0.33382 152B → 160B -0.26511 153B → 160B 0.77637 155B → 161B -0.10147	1.099
26	3.3022	375.46	0.0084	151A → 161A 0.10074 156A → 161A 0.22492 160A → 168A -0.12919 160A → 169A 0.14629 160A → 171A 0.52847 149B → 160B -0.16194 150B → 161B -0.12829 151B → 160B -0.40842 154B → 160B 0.51297 155B → 160B 0.21011 159B → 162B 0.10172	1.062
27	3.3406	371.14	0.0274	156A → 161A 0.57537 157A → 161A 0.30136 159A → 162A -0.29373 160A → 169A -0.24385 160A → 171A -0.30646 149B → 160B 0.11472 154B → 160B 0.19020 155B → 160B -0.17486 157B → 161B 0.31484 158B → 162B -0.12589 159B → 162B 0.29429	1.430

28	3.3747	367.39	0.3021	150A → 161A -0.12104 156A → 161A 0.37630 157A → 161A -0.14563 158A → 162A 0.12154 159A → 162A -0.33139 160A → 169A 0.32745 160A → 171A 0.36573 151B → 160B 0.49277 154B → 160B -0.24554 157B → 161B -0.18758 159B → 162B 0.23915	1.082
29	3.4229	362.22	0.0052	152A → 161A -0.10494 154A → 161A -0.10572 155A → 161A 0.56339 157A → 162A 0.14406 160A → 172A -0.11854 150B → 160B 0.46084 151B → 161B 0.12666 152B → 160B -0.38700 155B → 161B -0.20706 156B → 160B -0.21863 157B → 162B 0.17476	1.851
30	3.4264	361.85	0.7777	156A → 161A 0.31731 157A → 161A 0.13347 159A → 162A 0.55249 160A → 171A 0.37692 149B → 160B 0.12888 151B → 160B 0.23869 155B → 160B -0.16836 157B → 161B 0.38999 159B → 162B -0.34950	0.977

Table S18. 30 D3-B3LYP TDA transitions of **RC** at the D3-B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	1.0600	1169.67	0.5013	160A → 161A 0.95570 158B → 160B -0.17944 159B → 160B -0.13749	0.785
2	1.6405	755.78	0.0000	160A → 162A 0.97141	0.830
3	1.8784	660.04	0.1839	157A → 161A -0.14725 160A → 161A 0.10793 160A → 164A 0.10158 158B → 160B -0.14550 159B → 160B 0.94262	0.871

4	2.1254	583.34	0.0001	159A → 161A 0.70642 160A → 162A -0.13515 160A → 163A -0.17287 157B → 160B -0.44458 159B → 161B -0.44591	2.167
5	2.3155	535.46	0.6271	157A → 161A -0.14434 159A → 162A -0.11876 160A → 161A 0.16537 160A → 164A -0.10433 158B → 160B 0.91914 159B → 160B 0.10194 159B → 162B 0.12143	0.895
6	2.3456	528.57	0.0001	158A → 161A -0.11482 159A → 161A 0.28267 160A → 163A 0.89988 157B → 160B 0.16428 158B → 161B 0.13512	1.000
7	2.5918	478.38	0.0048	158A → 161A 0.78202 159A → 161A -0.20623 160A → 163A 0.29086 160A → 166A -0.10271 152B → 160B 0.11032 156B → 160B -0.15761 157B → 160B -0.28624 158B → 161B -0.30520	2.046
8	2.6554	466.91	0.0061	158A → 161A 0.33984 159A → 161A 0.11335 160A → 163A -0.14606 157B → 160B 0.75463 159B → 161B -0.46016	1.343
9	2.6836	462.01	0.0371	157A → 161A 0.34054 158A → 162A 0.11190 159A → 162A 0.14246 160A → 164A 0.75317 160A → 165A -0.18974 157B → 161B -0.23851 158B → 160B 0.16574 158B → 162B 0.17907 159B → 162B 0.21000	1.393
10	2.7457	451.56	0.0535	157A → 161A -0.30123 159A → 162A -0.11846 160A → 164A 0.50650 160A → 165A 0.57119 160A → 171A -0.12822 149B → 160B 0.13308 155B → 160B 0.34064 157B → 161B 0.25027 159B → 160B -0.12127 159B → 162B -0.13760	1.243

11	2.7787	446.19	0.0251	155A → 161A -0.11810 159A → 161A 0.47498 160A → 166A 0.33312 160A → 167A -0.19222 160A → 172A -0.13035 156B → 160B -0.26085 157B → 160B 0.13225 158B → 161B -0.30131 159B → 161B 0.61239	0.951
12	2.8161	440.27	0.0835	157A → 161A 0.29279 159A → 162A 0.10541 160A → 164A -0.22981 160A → 165A 0.75284 160A → 169A -0.11746 151B → 160B 0.12824 155B → 160B -0.21124 157B → 161B -0.26316 159B → 160B 0.12991 159B → 162B 0.26175	1.279
13	2.8216	439.41	0.0017	158A → 161A 0.12701 159A → 161A -0.17554 160A → 166A 0.88000 152B → 160B -0.12921 156B → 160B 0.13478 158B → 161B 0.15458 159B → 161B -0.14406	0.868
14	3.0050	412.60	0.0984	159A → 162A 0.45193 159A → 163A 0.16748 160A → 164A -0.17314 160A → 168A -0.36835 160A → 171A -0.15033 155B → 160B 0.52097 159B → 162B 0.42087 159B → 163B -0.11141	1.773
15	3.0221	410.26	0.0036	158A → 161A 0.10946 151B → 161B 0.11560 152B → 160B 0.10494 156B → 160B 0.86778 157B → 160B 0.12840 157B → 162B 0.10561 158B → 161B -0.22869 159B → 161B 0.25212	1.052

16	3.0254	409.81	0.0879	156A → 161A -0.15196 157A → 161A -0.44259 158A → 162A -0.20101 159A → 162A 0.28434 160A → 164A 0.13848 160A → 168A 0.23172 155B → 160B -0.40384 157B → 161B 0.17571 158B → 162B -0.17434 159B → 160B -0.11597 159B → 162B 0.49053 159B → 163B -0.11847	2.085
17	3.0595	405.24	0.0001	158A → 161A -0.25433 160A → 167A 0.81485 160A → 170A -0.11661 152B → 160B 0.13261 153B → 160B -0.13755 156B → 160B -0.13010 157B → 160B 0.11865 158B → 161B -0.34738	0.847
18	3.1272	396.46	0.0003	157A → 161A 0.43677 160A → 168A 0.34302 160A → 169A 0.74630 160A → 171A -0.14753 151B → 160B -0.15339 157B → 161B 0.16671	0.925
19	3.1672	391.46	0.0058	151A → 161A -0.10979 156A → 161A -0.19918 158A → 162A -0.14365 160A → 165A -0.13818 150B → 161B 0.17638 151B → 160B 0.42027 154B → 160B 0.72197 155B → 160B 0.11734 156B → 161B 0.17646 158B → 162B -0.16868 159B → 162B -0.15353	1.239
20	3.1958	387.96	0.0022	149A → 161A -0.10370 152A → 161A -0.15574 155A → 161A -0.19819 160A → 166A 0.20955 160A → 167A 0.19928 160A → 172A -0.19194 150B → 160B 0.41114 151B → 161B 0.16512 152B → 160B 0.29519 153B → 160B 0.58255 155B → 161B 0.14145 158B → 161B 0.28713	1.185

21	3.2279	384.10	0.0043	158A → 162A -0.10006 159A → 162A 0.15169 160A → 168A 0.72402 160A → 169A -0.34246 149B → 160B -0.10140 154B → 160B -0.12657 155B → 160B 0.44431 157B → 161B -0.15700 158B → 162B -0.15780	0.984
22	3.2387	382.83	0.0096	157A → 162A -0.11263 158A → 161A 0.26474 159A → 161A 0.17138 160A → 167A 0.28403 160A → 170A 0.28901 152B → 160B 0.20189 153B → 160B -0.49740 158B → 161B 0.57389 159B → 161B 0.18942	0.900
23	3.2946	376.32	0.0206	156A → 161A 0.26340 157A → 161A -0.16644 158A → 162A 0.42086 160A → 168A 0.28719 160A → 169A -0.10790 149B → 160B 0.16777 151B → 160B -0.22036 154B → 160B 0.47211 155B → 160B -0.10237 158B → 162B 0.47400	1.827
24	3.2956	376.21	0.0002	160A → 167A 0.10335 160A → 170A 0.89138 160A → 172A 0.12815 152B → 160B -0.23212 153B → 160B 0.14266 158B → 161B -0.23757	0.876
25	3.3226	373.16	0.0103	156A → 161A 0.16906 158A → 162A -0.14421 160A → 168A -0.11356 160A → 169A 0.14660 160A → 171A 0.60292 149B → 160B -0.21848 150B → 161B -0.13597 151B → 160B -0.41441 154B → 160B 0.36530 155B → 160B 0.22847 157B → 161B -0.13550 158B → 162B -0.15588	1.099

26	3.3339	371.89	0.0103	152A → 161A 0.18808 154A → 161A 0.13601 155A → 161A 0.15557 158A → 161A 0.15175 159A → 161A 0.10384 160A → 166A -0.11304 160A → 167A 0.23373 160A → 172A 0.12551 150B → 160B -0.51423 151B → 161B -0.12313 152B → 160B -0.14332 153B → 160B 0.58106 155B → 161B -0.11540 158B → 161B 0.20089 159B → 161B 0.12844	1.062
27	3.3705	367.85	0.0092	156A → 161A 0.56166 157A → 161A 0.31186 158A → 162A -0.23360 159A → 162A -0.24189 160A → 168A -0.10791 160A → 169A -0.24298 160A → 171A -0.27000 154B → 160B 0.16197 155B → 160B -0.13495 157B → 161B 0.31726 158B → 162B -0.24810 159B → 162B 0.25596	1.430
28	3.4058	364.04	0.0412	150A → 161A -0.12939 156A → 161A 0.48286 158A → 162A 0.13668 160A → 169A 0.23522 160A → 171A 0.48054 149B → 160B 0.12271 150B → 161B 0.10825 151B → 160B 0.56446 154B → 160B -0.18746	1.082
29	3.4575	358.60	0.0068	155A → 161A 0.68221 157A → 162A 0.14870 160A → 172A -0.22005 150B → 160B 0.35140 151B → 161B 0.11168 152B → 160B -0.31975 155B → 161B -0.22417 156B → 160B -0.19816 157B → 160B 0.10062 157B → 162B 0.17198	1.851

30	3.4936	354.89	0.0034	152A → 161A -0.11545 154A → 161A -0.13084 155A → 161A 0.42111 157A → 162A 0.18455 160A → 167A -0.14728 160A → 170A 0.21278 160A → 172A -0.28096 150B → 160B -0.42526 152B → 160B 0.56419 157B → 162B -0.12159	0.977

Table S19. 30 D3-BLYP TDDFT transitions of **RC** at the TDDFT D3-BLYP D_4 optimized geometry (excited state 5 in Table S17).

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	1.0598	1169.92	0.2472	160A → 161A 0.95955 158B → 160B -0.23154	0.786
2	1.5355	807.43	0.0003	159A → 161A 0.12064 160A → 162A 0.94575 157B → 160B -0.12576 158B → 161B -0.16798 159B → 161B -0.12671	0.921
3	1.587	781.23	0.0543	157A → 161A -0.11319 158B → 160B -0.15678 159B → 160B 0.95965	0.850
4	1.8991	652.86	0.6024	160A → 161A 0.22360 158B → 160B 0.93679 159B → 160B 0.14045	0.826
5	2.046	605.98	0.0055	157A → 162A -0.10691 158A → 161A -0.17567 159A → 161A -0.52434 160A → 162A 0.24924 156B → 160B -0.12446 157B → 160B 0.63570 158B → 161B 0.14412 159B → 161B 0.37329	1.740
6	2.3828	520.33	0.0026	158A → 161A -0.39380 159A → 161A 0.47831 160A → 163A -0.40937 156B → 160B 0.22649 157B → 160B 0.42304 158B → 161B 0.24306 159B → 161B -0.33723	1.894
7	2.4558	504.87	0.0072	158A → 161A 0.64020 159A → 161A 0.11486 160A → 162A -0.12249 157B → 160B 0.55546 157B → 162B -0.13375	1.972

				158B → 161B -0.35454 159B → 161B -0.23460	
8	2.4849	498.96	0.0001	157A → 161A 0.42914 158A → 162A 0.31811 159A → 162A 0.23842 160A → 164A -0.29557 160A → 169A -0.11283 155B → 160B -0.32895 157B → 161B -0.37319 158B → 162B -0.34318 159B → 160B 0.13341 159B → 162B -0.27585	2.229
9	2.6024	476.42	0.0102	158A → 161A -0.25982 159A → 161A 0.15209 160A → 163A 0.87233 157B → 160B 0.23701 159B → 161B -0.17137	1.023
10	2.6884	461.18	0.0114	155A → 161A -0.10007 158A → 161A -0.14891 159A → 161A 0.57040 156B → 160B -0.56437 158B → 161B -0.20295 159B → 161B 0.48825	0.819
11	2.697	459.72	0.0724	158A → 162A -0.16633 160A → 164A 0.64251 151B → 161B -0.11722 155B → 160B -0.56813 156B → 161B 0.14349 158B → 162B 0.23794 159B → 162B -0.23288	1.178
12	2.7757	446.68	0.0076	159A → 161A 0.14530 156B → 160B 0.71836 158B → 161B -0.34914 159B → 161B 0.53425	1.094
13	2.8194	439.76	0.0359	157A → 161A 0.19396 158A → 162A 0.29943 159A → 162A 0.10556 160A → 164A 0.60095 160A → 165A 0.10396 154B → 160B -0.1363 155B → 160B 0.55582 157B → 161B -0.10622 158B → 162B -0.21718	1.293
14	2.8829	430.06	0.0047	158A → 162A 0.12418 159A → 162A -0.29126 160A → 165A 0.57074 150B → 161B -0.10580 152B → 160B -0.32243 154B → 160B -0.33208 155B → 160B -0.22663	1.539

				158B → 162B -0.13979 159B → 162B 0.43472	
15	2.9156	425.25	0.0000	152A → 161A -0.10228 158A → 161A 0.12675 160A → 166A 0.77042 150B → 160B -0.18762 151B → 160B -0.26428 152B → 161B -0.13502 153B → 160B -0.35049 158B → 161B 0.16960	0.979
16	2.9349	422.44	0.0385	158A → 162A -0.28476 159A → 162A 0.36603 160A → 164A -0.18989 160A → 165A 0.66682 155B → 160B 0.29168 158B → 162B 0.27730 159B → 162B -0.27182	1.556
17	2.9895	414.73	0.0190	158A → 161A 0.39059 159A → 161A 0.20519 160A → 166A 0.18050 160A → 167A 0.22968 150B → 160B 0.12740 151B → 160B 0.21387 153B → 160B 0.43030 156B → 160B 0.12836 158B → 161B 0.58980 159B → 161B 0.21937	0.858
18	3.0014	413.09	0.0109	159A → 162A -0.10530 160A → 164A 0.12883 160A → 165A 0.28185 152B → 160B 0.13067 154B → 160B 0.86688 159B → 162B 0.27430	0.986
19	3.0299	409.21	0.0058	158A → 161A -0.21094 159A → 161A -0.13126 160A → 166A 0.36540 151B → 160B -0.19618 153B → 160B 0.77369 158B → 161B -0.33700 159B → 161B -0.10703	0.817

20	3.0748	403.23	0.0636	157A → 161A 0.48829 158A → 162A -0.26582 159A → 162A -0.23152 159A → 163A 0.13560 160A → 165A -0.15364 160A → 169A -0.19586 149B → 160B 0.19565 152B → 160B 0.16971 154B → 160B -0.11101 155B → 160B 0.17705 155B → 162B -0.12816 157B → 161B -0.32755 158B → 160B 0.12448 158B → 162B 0.30296 159B → 162B 0.31361 159B → 163B -0.17803	2.289
21	3.1288	396.26	0.0008	152A → 161A 0.12031 157A → 162A 0.12166 158A → 161A -0.16771 160A → 166A 0.34334 160A → 167A -0.43412 160A → 170A -0.14851 160A → 172A 0.14769 150B → 160B 0.22893 151B → 160B 0.64298 152B → 161B 0.14160	1.036
22	3.141	394.73	0.0063	157A → 161A -0.21282 158A → 162A 0.11883 160A → 165A 0.18519 160A → 169A -0.12940 150B → 161B 0.13020 151B → 161B 0.12590 152B → 160B 0.80093 154B → 160B -0.27832 155B → 160B -0.14054 159B → 162B 0.13641	1.077
23	3.1845	389.33	0.0043	160A → 166A 0.19138 160A → 167A 0.53568 160A → 170A 0.16372 150B → 160B 0.64920 152B → 161B 0.10106 153B → 160B -0.25414 157B → 162B 0.10358 158B → 161B -0.19249	0.979

24	3.2099	386.26	0.2783	156A → 161A -0.15663 157A → 161A 0.43327 159A → 162A 0.32319 160A → 169A 0.58392 160A → 171A -0.16562 149B → 160B -0.26166 154B → 160B -0.12219 157B → 161B 0.20195 159B → 162B 0.29091	1.014
25	3.2384	382.86	0.5592	156A → 161A -0.15637 157A → 161A -0.26658 158A → 162A -0.10681 159A → 162A 0.64206 160A → 165A -0.14382 160A → 169A -0.30479 149B → 160B 0.14777 152B → 160B -0.10538 157B → 161B -0.10601 158B → 162B -0.14093 159B → 162B 0.50812	0.860
26	3.3038	375.28	0.0118	155A → 161A 0.21812 160A → 166A -0.12303 160A → 167A -0.39846 150B → 160B 0.56579 151B → 160B -0.36035 155B → 161B -0.23571 156B → 160B -0.12192 156B → 162B 0.10905 157B → 162B -0.31265 158B → 161B 0.12025 159B → 161B 0.14849	1.256
27	3.3151	374	0.0166	157A → 161A -0.24921 158A → 162A 0.14189 159A → 163A 0.11380 160A → 168A 0.74499 160A → 169A 0.27195 160A → 171A 0.15460 152B → 160B 0.11883 155B → 160B 0.15735 156B → 161B 0.11015 157B → 161B -0.27743	1.054

28	3.3633	368.64	0.0005	149A → 161A 0.12343 155A → 161A -0.38299 157A → 162A -0.33713 159A → 164A 0.11361 160A → 166A 0.10603 160A → 167A -0.45717 160A → 170A 0.52763 160A → 172A -0.12629 150B → 160B 0.12298 151B → 160B -0.15622 155B → 161B 0.13314 157B → 162B 0.19096	1.506
29	3.368	368.12	0.0586	150A → 161A 0.10005 156A → 161A -0.42329 157A → 161A -0.10466 159A → 162A -0.17273 160A → 168A -0.17764 160A → 169A 0.35417 148B → 160B -0.10863 149B → 160B 0.68506 156B → 161B 0.11258	1.313
30	3.4142	363.15	0.1539	156A → 161A 0.53773 157A → 161A 0.20657 159A → 162A 0.17008 160A → 168A 0.32025 149B → 160B 0.45752 152B → 160B 0.14055 157B → 161B 0.48973	1.303

B. B3LYP

Table S20. 30 CIS transitions of **RC** at the B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	1.0621	1167.37	0.5025	160A → 161A 0.95503 158B → 160B 0.17653 159B → 160B -0.14608	0.785
2	1.6308	760.27	0.0000	160A → 162A 0.97247	0.829
3	1.8860	657.40	0.1991	157A → 161A -0.14930 160A → 161A 0.11486 160A → 164A -0.10199 158B → 160B 0.15266 159B → 160B 0.93997	0.873
4	2.1275	582.78	0.0001	159A → 161A 0.70613 160A → 162A 0.13204 160A → 163A -0.17421 157B → 160B -0.44434 159B → 161B -0.45018	2.172
5	2.3240	533.49	0.6247	157A → 161A 0.13717 159A → 162A -0.11665 160A → 161A -0.16414 160A → 164A -0.10801 158B → 160B 0.91847 159B → 160B -0.10962 159B → 162B -0.12692	0.892
6	2.3578	525.84	0.0001	158A → 161A 0.11618 159A → 161A 0.28566 160A → 163A 0.89829 157B → 160B 0.16486 158B → 161B -0.13677	1.001
7	2.6069	475.61	0.0042	158A → 161A 0.79817 159A → 161A 0.17436 160A → 163A -0.28246 160A → 166A -0.10461 152B → 160B -0.11766 156B → 160B 0.16998 157B → 160B 0.24893 158B → 161B -0.31490	2.086
8	2.6607	465.98	0.0071	158A → 161A -0.30192 159A → 161A 0.13638 160A → 163A -0.15991 160A → 167A -0.10015 157B → 160B 0.77075 159B → 161B -0.44771	1.318

9	2.6889	461.10	0.0350	157A → 161A -0.34736 158A → 162A -0.11163 159A → 162A 0.15648 160A → 164A 0.73950 160A → 165A -0.18778 157B → 161B 0.24213 158B → 160B 0.16170 158B → 162B 0.17922 159B → 162B -0.23024	1.431
10	2.7481	451.17	0.0522	157A → 161A 0.30004 159A → 162A -0.12598 160A → 164A 0.52148 160A → 165A 0.56007 160A → 171A -0.13014 149B → 160B -0.13913 155B → 160B -0.33146 157B → 161B -0.25169 159B → 160B 0.12070 159B → 162B 0.14047	1.247
11	2.7888	444.58	0.0242	155A → 161A 0.10135 159A → 161A 0.45427 160A → 166A -0.42610 160A → 167A -0.19390 160A → 172A -0.12492 156B → 160B -0.24953 157B → 160B 0.10697 158B → 161B 0.27618 159B → 161B 0.59537	0.922
12	2.8217	439.40	0.0763	157A → 161A -0.27858 159A → 162A 0.11228 160A → 164A -0.23347 160A → 165A 0.76181 160A → 169A -0.11701 151B → 160B -0.13197 155B → 160B 0.20225 157B → 161B 0.25650 159B → 160B -0.12825 159B → 162B -0.26451	1.260
13	2.8234	439.13	0.0034	155A → 161A 0.10690 158A → 161A 0.13936 159A → 161A 0.22529 160A → 166A 0.83891 160A → 172A -0.10939 152B → 160B 0.13385 156B → 160B -0.15766 157B → 160B 0.10246 158B → 161B 0.17693 159B → 161B 0.21264	0.871

14	3.0007	413.19	0.1376	157A → 161A -0.12320 159A → 162A -0.49923 159A → 163A 0.17426 160A → 164A 0.14596 160A → 168A 0.29582 160A → 169A -0.12145 160A → 171A 0.13493 155B → 160B 0.41904 159B → 162B 0.51418 159B → 163B -0.13335	2.060
15	3.0288	409.36	0.0565	156A → 161A 0.15089 157A → 161A 0.40903 158A → 162A 0.21203 159A → 162A 0.17225 160A → 164A 0.17386 160A → 168A 0.33883 160A → 171A 0.10957 155B → 160B 0.50402 157B → 161B -0.16567 158B → 162B -0.19547 159B → 160B 0.10538 159B → 162B -0.38698	1.770
16	3.0313	409.01	0.0039	158A → 161A -0.12820 150B → 160B 0.10266 151B → 161B 0.12156 152B → 160B 0.10686 156B → 160B 0.87160 157B → 160B 0.11863 157B → 162B 0.10557 158B →161B 0.20455 159B → 161B 0.25810	1.042
17	3.0625	404.85	0.0002	158A → 161A 0.24922 160A → 167A 0.82210 160A → 170A -0.10869 152B → 160B 0.14789 153B → 160B -0.12745 157B → 160B 0.12574 158B → 161B 0.35011	0.849
18	3.1273	396.46	0.0005	157A → 161A -0.45314 160A → 168A 0.43570 160A → 169A 0.68381 160A → 171A -0.16377 151B → 160B 0.16830 157B → 161B -0.14639	0.942

19	3.1685	391.31	0.0049	151A → 161A 0.11620 156A → 161A 0.20546 158A → 162A 0.16018 160A → 165A -0.13821 150B → 161B -0.17902 151B → 160B -0.44010 154B → 160B 0.69505 155B → 160B -0.13839 156B → 161B -0.18096 158B → 162B -0.18808 159B → 162B 0.13856	1.264
20	3.1979	387.70	0.0018	149A → 161A -0.10820 152A → 161A -0.15868 155A → 161A 0.19388 160A → 166A -0.20986 160A → 167A 0.17177 160A → 172A -0.20076 149B → 161B 0.10669 150B → 160B 0.42975 151B → 161B 0.16437 152B → 160B 0.29402 153B → 160B 0.57404 155B → 161B 0.14467 158B → 161B -0.29262	1.193
21	3.2287	384.00	0.0048	156A → 161A -0.10226 159A → 162A 0.14829 160A → 168A 0.66609 160A → 169A -0.44497 149B → 160B 0.10954 154B → 160B -0.15208 155B → 160B -0.44801 157B → 161B 0.16333 158B → 162B -0.13953	0.957
22	3.2424	382.38	0.0086	157A → 162A -0.11024 158A → 161A 0.25568 159A → 161A -0.17176 160A → 167A -0.27163 160A → 170A -0.28808 152B → 160B -0.20798 153B → 160B 0.50501 158B → 161B 0.57789 159B → 161B -0.18909	0.906
23	3.2909	376.75	0.0165	156A → 161A -0.24064 157A → 161A 0.17149 158A → 162A -0.41298 160A → 168A 0.25707 160A → 169A -0.14817 149B → 160B -0.16270 151B → 160B 0.22599 154B → 160B 0.51221 158B → 162B 0.46805	1.774

24	3.2964	376.12	0.0002	160A → 170A 0.90245 160A → 172A 0.12022 152B → 160B -0.20692 153B → 160B 0.13458 158B → 161B 0.23588	0.868
25	3.3200	373.45	0.0101	156A → 161A -0.15509 158A → 162A 0.16014 160A → 168A -0.10627 160A → 169A 0.16140 160A → 171A 0.58254 149B → 160B 0.24027 150B → 161B 0.13971 151B → 160B 0.41295 154B → 160B 0.36069 155B → 160B -0.24895 157B → 161B 0.13218 158B → 162B -0.17301	1.115
26	3.3294	372.39	0.0101	152A → 161A 0.18805 154A → 161A -0.11962 155A → 161A -0.14380 158A → 161A -0.15465 159A → 161A 0.10973 160A → 166A 0.10936 160A → 167A 0.24445 160A → 172A 0.12812 150B → 160B -0.51140 151B → 161B -0.12295 152B → 160B -0.12861 153B → 160B 0.58796 155B → 161B -0.10557 158B → 161B -0.21342 159B → 161B 0.13310	1.041
27	3.3727	367.61	0.0126	156A → 161A 0.50561 157A → 161A 0.31465 158A → 162A -0.23982 159A → 162A 0.24841 160A → 168A 0.12618 160A → 169A 0.25466 160A → 171A 0.33651 151B → 160B -0.12004 154B → 160B -0.18258 155B → 160B -0.12001 157B → 161B 0.29403 158B → 162B 0.25561 159B → 162B 0.25277	1.386

28	3.4029	364.35	0.0521	150A → 161A -0.12608 156A → 161A 0.55247 158A → 162A 0.11886 159A → 162A 0.12674 160A → 169A -0.21360 160A → 171A -0.45529 149B → 160B 0.13480 150B → 161B 0.10377 151B → 160B 0.52999 154B → 160B 0.15842 159B → 162B 0.11402	1.141
29	3.4600	358.33	0.0075	155A → 161A 0.63346 157A → 162A 0.12893 160A → 167A -0.10816 160A → 172A 0.19700 150B → 160B -0.38098 151B → 161B -0.11228 152B → 160B 0.39315 155B → 161B 0.22239 156B → 160B 0.19072 157B → 160B -0.10144 157B → 162B -0.18959	1.750
30	3.4922	355.03	0.0030	152A → 161A -0.12504 154A → 161A 0.13552 155A → 161A -0.48389 157A → 162A -0.20407 160A → 167A -0.14674 160A → 170A 0.19864 160A → 172A -0.32328 150B → 160B -0.38506 152B → 160B 0.52227 157B → 162B -0.10035	1.065

Table S21. 30 B3LYP TDDFT calculated transitions of **RC** at the B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	0.9538	1299.83	0.3172	160A → 161A 0.97808 158B → 160B 0.13539 159B → 160B -0.12085	0.777
2	1.6045	772.72	0.0014	159A → 161A -0.13470 160A → 162A 0.95324 158B → 161B 0.10002 159B → 160B 0.11905 159B → 161B -0.13665	0.876

3	1.7921	691.85	0.1292	157A → 161A -0.14158 160A → 161A 0.11253 160A → 162A -0.11656 157B → 161B -0.11144 158B → 160B 0.10501 159B → 160B 0.94207	0.879
4	2.0836	595.05	0.0033	158A → 161A -0.13804 159A → 161A 0.66824 160A → 162A 0.22003 160A → 163A 0.12384 157B → 160B -0.41663 158B → 160B -0.12478 158B → 161B -0.12145 159B → 161B 0.45147	2.196
5	2.2552	549.76	0.3660	157A → 161A 0.10490 158A → 161A 0.17810 159A → 161A 0.11048 159A → 162A -0.10858 160A → 161A -0.13610 157B → 160B -0.10815 157B → 161B 0.10380 158B → 160B 0.90066	1.069
6	2.3633	524.63	0.0021	158A → 161A -0.12829 159A → 161A -0.26724 160A → 163A 0.89846 157B → 160B -0.19125 158B → 161B -0.11380	0.972
7	2.5732	481.84	0.0419	157A → 161A 0.15091 158A → 161A 0.53856 158A → 162A 0.11805 159A → 161A 0.29913 160A → 163A 0.28355 160A → 164A -0.16913 160A → 165A 0.27985 160A → 167A -0.10736 151B → 160B -0.10216 157B → 160B 0.37363 157B → 161B 0.13372 158B → 160B -0.16942 158B → 161B 0.25281 158B → 162B -0.12239 159B → 160B 0.12911 159B → 162B 0.14545	1.801

8	2.6640	465.41	0.0080	157A → 161A -0.29659 158A → 161A 0.58355 159A → 162A 0.11485 160A → 165A -0.21878 154B → 160B -0.10643 155B → 160B 0.14411 157B → 160B -0.39753 157B → 161B -0.17947 158B → 161B 0.14842 159B → 161B -0.35728 159B → 162B -0.12593	1.820
9	2.6795	462.71	0.0455	157A → 161A 0.18764 158A → 161A 0.11677 158A → 162A 0.11390 159A → 161A -0.14340 160A → 164A 0.76471 160A → 165A -0.23232 160A → 166A 0.10709 152B → 160B 0.12162 156B → 160B -0.10828 157B → 161B 0.15516 158B → 160B -0.14259 158B → 162B -0.12722 159B → 161B 0.21605 159B → 162B 0.18005	1.106
10	2.7119	457.18	0.0053	157A → 161A -0.26127 158A → 162A -0.10504 159A → 162A 0.14583 160A → 163A 0.19089 160A → 165A -0.43523 160A → 169A -0.13284 155B → 160B 0.15376 157B → 160B 0.55712 157B → 161B -0.22987 158B → 160B 0.11949 158B → 162B 0.11715 159B → 161B 0.36863 159B → 162B -0.15940	1.311
11	2.7402	452.46	0.0310	158A → 161A 0.13233 159A → 161A -0.48986 160A → 163A -0.11640 160A → 164A -0.37026 160A → 173A -0.11083 151B → 160B -0.11118 156B → 160B -0.20135 157B → 160B -0.25121 158B→ 161B 0.29154 159B → 161B 0.53186	1.002

12	2.8094	441.32	0.0654	157A → 161A -0.22553 159A → 161A -0.16360 160A → 164A 0.31270 160A → 165A 0.72962 154B → 160B -0.12322 155B → 160B 0.22180 156B → 160B -0.11050 157B → 161B -0.21242 159B → 160B -0.11238 159B → 161B 0.16888 159B → 162B -0.16367	1.115
13	2.9452	420.97	0.0114	158A → 161A 0.10134 160A → 166A 0.91767 151B → 160B 0.12330 156B → 160B 0.11974 159B → 162B -0.14455	0.903
14	2.9760	416.61	0.0165	158A → 161A 0.10186 158A → 162A 0.10864 159A → 162A 0.15169 160A → 164A 0.10573 160A → 166A -0.13030 152B → 160B -0.22977 152B → 161B 0.14218 156B → 160B 0.79894 156B → 161B -0.17128 158B → 162B -0.12383 159B → 161B 0.20976 159B → 162B -0.19916	1.123
15	3.0190	410.68	0.0334	158A → 161A 0.14040 158A → 162A -0.17673 159A → 162A 0.19206 159A → 163A 0.10671 160A → 164A 0.13870 160A → 165A 0.16149 160A → 167A 0.60501 160A → 170A -0.21391 155B → 160B -0.50851 157B → 160B 0.10384 158B → 161B -0.15099 158B → 162B 0.17104 159B → 162B -0.10405	1.166
16	3.0741	403.32	0.0969	157A → 161A -0.27575 159A → 162A -0.40780 159A → 163A -0.12504 160A → 166A 0.10604 160A → 167A 0.19967 160A → 168A 0.22443 156B → 160B 0.25125 157B → 161B -0.14757 159B → 162B 0.62692 159B → 163B 0.14061	2.211

17	3.0912	401.09	0.0065	157A → 161A 0.23281 158A → 161A 0.15530 158A → 162A 0.11909 160A → 167A 0.36355 160A → 168A 0.41862 160A → 169A 0.29629 153B → 160B -0.12538 154B → 160B -0.15024 155B → 160B 0.40147 156B → 160B -0.13081 157B → 160B 0.10249 157B → 161B 0.10218 158B → 161B -0.32062 158B → 162B -0.11662 159B → 162B -0.13910	1.177
18	3.1316	395.92	0.0068	160A → 164A 0.19568 160A → 165A -0.10977 160A → 167A -0.43005 160A → 168A 0.44635 152B → 160B -0.29263 154B → 160B -0.36064 155B → 160B -0.38407 156B → 160B -0.16943	0.984
19	3.1497	393.63	0.0004	157A → 161A -0.34535 158A → 162A -0.13766 160A → 167A -0.25528 160A → 168A -0.29277 160A → 169A 0.70316 160A → 170A -0.14702 150B → 160B -0.13008 154B → 160B -0.10109 157B → 161B 0.11068 158B → 161B -0.22839	1.002
20	3.1545	393.04	0.0121	156A → 161A -0.14667 158A → 161A 0.24910 158A → 162A -0.21202 160A → 166A -0.12530 160A → 167A -0.33876 160A → 168A 0.46531 160A → 170A -0.10590 152B → 160B 0.15583 154B → 160B 0.47061 156B → 160B 0.12549 156B → 161B 0.10233 158B → 161B -0.21334 158B → 162B 0.20072 159B → 161B 0.15554	1.201

21	3.2170	385.41	0.0151	157A → 161A -0.29928 158A → 161A -0.16883 158A → 162A 0.19695 159A → 161A 0.10927 160A → 168A 0.33484 160A → 169A 0.37964 160A → 173A 0.11073 151B → 160B 0.28242 152B → 160B 0.11413 154B → 160B 0.22352 155B → 160B -0.19515 158B → 161B 0.45911 158B → 162B -0.22291	1.341
22	3.2622	380.06	0.0132	157A → 161A 0.18183 158A → 161A -0.21209 158A → 162A -0.29730 159A → 161A 0.11409 160A → 164A 0.10083 160A → 166A 0.11298 160A → 168A 0.18423 160A → 170A -0.25435 150B → 160B -0.15474 151B → 160B -0.13822 152B → 160B -0.17376 155B → 160B 0.33080 158B → 160B -0.10274 158B → 161B 0.47638 158B → 162B 0.32940 159B → 161B -0.12325 159B → 163B -0.11837	1.462
23	3.2911	376.72	0.0131	149A → 161A 0.11575 151A → 161A 0.11204 153A → 161A 0.10498 156A → 161A 0.11587 157A → 161A -0.10349 158A → 162A 0.12576 160A → 169A -0.10685 160A → 170A -0.26268 149B → 160B -0.24638 149B → 161B -0.14302 150B → 160B 0.11911 151B → 160B 0.10253 152B → 160B -0.38642 153B → 160B 0.57142 154B → 160B 0.16281 155B → 160B 0.26258 156B → 160B -0.14794 158B → 162B -0.13869	1.188

24	3.2988	375.84	0.0084	152A → 161A 0.10064 157A → 161A -0.19581 158A → 162A 0.13974 149B → 160B 0.18588 151B → 160B -0.19887 152B → 160B -0.37380 152B → 161B 0.11339 153B → 160B -0.49287 154B → 160B 0.52283 156B → 160B -0.19448 158B → 162B -0.17387	1.105
25	3.3812	366.68	0.0337	155A → 161A -0.11038 157A → 161A 0.28386 158A → 162A -0.22263 160A → 168A -0.12959 160A → 169A 0.20462 160A → 170A 0.48523 149B → 160B -0.15838 151B → 160B 0.28831 152B → 160B -0.43182 153B → 160B -0.14098 154B → 160B 0.11317 156B → 160B -0.10604 157B → 161B -0.23620 158B → 162B 0.17782	1.153
26	3.3906	365.67	0.2357	154A → 161A -0.12501 156A → 161A 0.47361 157A → 161A 0.13451 159A → 162A 0.52890 160A → 170A 0.23778 149B → 160B 0.11786 151B → 160B -0.17537 152B → 160B 0.14532 153B → 160B 0.19129 154B → 160B 0.23444 157B → 161B -0.13374 159B → 162B 0.37260	1.126
27	3.4060	364.02	0.0612	154A → 161A 0.13285 155A → 161A 0.13692 156A → 161A -0.40022 159A → 162A -0.10790 160A → 169A 0.12771 160A → 170A 0.40692 160A → 173A -0.10889 149B → 160B 0.18237 151B → 160B -0.33811 152B → 160B -0.17520 153B → 160B 0.47060 159B → 162B -0.18907	1.208

28	3.4596	358.38	0.6292	156A → 161A -0.53820 157A → 161A -0.13743 159A → 162A 0.54445 160A → 170A 0.10889 152B → 160B -0.17062 153B → 160B -0.15280 154B → 160B -0.13766 155B → 160B 0.13952 157B → 161B 0.31579 159B → 162B 0.31851	1.264
29	3.4880	355.46	0.0111	153A → 161A 0.13776 154A → 161A 0.17899 155A → 161A -0.31476 156A → 161A 0.13516 157A → 162A 0.17241 160A → 168A 0.14555 160A → 170A 0.25302 160A → 171A 0.67512 160A → 173A -0.13600 150B → 160B -0.14111 151B → 160B -0.15722 152B → 160B 0.11144 154B → 160B -0.13071 157B → 162B -0.11746	1.276
30	3.5139	352.84	0.0199	151A → 161A 0.15362 154A → 161A -0.22741 155A → 161A 0.51583 156A → 161A -0.10278 157A → 162A -0.11690 159A → 162A -0.10399 160A → 170A 0.14000 160A → 171A 0.42917 149B → 160B -0.26652 150B → 160B 0.33334 151B → 160B -0.10827 152B → 160B 0.12049 153B → 160B -0.13369 154B → 160B 0.15995 154B → 161B -0.10360 155B → 161B 0.14279 157B → 162B 0.12381	1.613

C. CAM-B3LYP

Table S22. 30 CIS transitions of **RC** at the CAM-B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	1.0661	1163.00	0.5261	160A → 161A 0.96952 158B → 160B 0.10389	0.848
2	1.9306	642.20	0.0000	159A → 161A 0.22892 160A → 162A 0.91249 160A → 163A 0.13254 159B → 161B -0.13297	1.045
3	2.2827	543.16	0.1791	157A → 161A 0.18825 157B → 161B -0.23641 158B → 162B -0.11616 159B→ 160B 0.89543	1.133
4	2.4644	503.09	0.0001	157A → 162A 0.11009 159A → 161A 0.61987 160A → 162A -0.25427 160A → 163A -0.24791 157B → 160B 0.43259 159B → 161B -0.42967	2.053
5	2.7099	457.53	0.5418	157A → 161A 0.13254 159A → 162A 0.10976 160A → 164A -0.16369 152B → 161B 0.15201 156B → 161B -0.14768 157B → 161B -0.16365 158B → 160B 0.86603 159B → 163B 0.10653	1.137
6	2.7618	448.92	0.0000	158A → 161A -0.52059 159A → 161A 0.22538 160A → 162A -0.13322 160A → 163A 0.65664 152B → 160B 0.11821 156B → 160B -0.17910 158B → 161B 0.25238	1.623
7	3.0013	413.11	0.0322	157A → 161A 0.38792 158A → 162A 0.15392 159A → 162A 0.29768 160A → 164A -0.36324 160A → 165A 0.14685 160A → 168A 0.15509 148B → 160B 0.11661 151B → 160B 0.15906 155B → 160B 0.22947 157B → 161B -0.26993 158B → 160B -0.19389 158B → 162B -0.17196	2.036

				159B → 160B -0.17720 159B → 162B -0.38513	
8	3.0823	402.25	0.0040	158A → 161A 0.61964 160A → 162A -0.15780 160A → 163A 0.58609 160A → 166A 0.19536 152B → 160B -0.12805 156B → 160B 0.12959 158B → 161B -0.23077	1.680
9	3.2085	386.42	0.0591	149A → 161A -0.14245 155A → 161A 0.17035 159A → 161A 0.58201 160A → 163A -0.10468 160A → 166A -0.14193 160A → 167A -0.16069 155B → 161B 0.15772 156B → 160B 0.25045 157B → 160B -0.50636 158B → 161B -0.12397 159B → 161B 0.30184	1.171
10	3.2138	385.79	0.0774	150A → 161A 0.13845 158A → 162A -0.20148 160A → 164A 0.61482 160A → 165A 0.22833 160A → 172A 0.18109 149B → 160B 0.17711 150B → 161B -0.10531 152B → 161B -0.11629 155B → 160B 0.33025 156B → 161B 0.15024 157B → 161B -0.17088 158B → 160B 0.11482 158B → 162B 0.26799 159B → 162B -0.21125	1.482
11	3.3336	371.92	0.0597	150A → 161A 0.10333 158A → 162A 0.12635 159A → 163A -0.12466 159A → 166A -0.14135 160A → 165A 0.66804 160A → 172A 0.15729 150B → 161B -0.15496 151B → 160B -0.21431 154B → 160B 0.12083 156B → 161B -0.10408 158B → 162B -0.13124 159B → 162B 0.41708 159B → 163B 0.10870	1.570

12	3.3556	369.48	0.0002	149A → 161A -0.14652 155A → 161A 0.11392 158A → 161A -0.24096 158A → 165A -0.12098 159A → 165A -0.15949 160A → 163A -0.15699 160A → 166A 0.73853 160A → 170A -0.12667 160A → 171A 0.12936 149B → 161B 0.13313 150B → 160B -0.21016 151B → 161B -0.11342 152B → 160B -0.13300 153B → 160B -0.10514 155B → 161B 0.11352	1.325
13	3.4587	358.47	0.3308	157A → 161A -0.19023 157A → 164A -0.10006 159A → 162A 0.29288 159A → 163A 0.24974 160A → 165A 0.40846 160A → 169A 0.23816 151B → 162B 0.11075 155B → 160B -0.27097 156B → 161B -0.12194 157B → 161B 0.12662 158B → 160B 0.12057 159B → 160B 0.14220 159B → 162B -0.38824 159B → 163B -0.27393	1.998
14	3.4658	357.74	0.0021	158A → 161A -0.33322 160A → 163A 0.11518 160A → 167A 0.15349 149B → 161B -0.12763 150B → 160B 0.21108 156B → 160B 0.45263 157B → 160B 0.41934 157B → 162B 0.15813 158B → 161B -0.40986 159B → 161B 0.31591	1.078

15	3.5396	350.28	0.1076	151A → 161A -0.14043 156A → 161A 0.26117 157A → 161A 0.14538 158A → 162A 0.25942 158A → 163A -0.18571 159A → 167A 0.12101 160A → 164A 0.44759 160A → 165A -0.16739 160A → 168A 0.40340 160A → 169A -0.13006 148B → 160B 0.15287 152B → 161B 0.11272 155B → 160B -0.18827 156B → 161B -0.16040 158B → 162B -0.21550 158B → 163B 0.15384 159B → 160B -0.14174	1.770
16	3.6396	340.66	0.0046	148A → 161A 0.10892 152A → 161A 0.14774 157A → 162A 0.15954 158A → 161A -0.18052 158A → 164A -0.13220 159A → 168A 0.16403 160A → 166A -0.24431 160A → 167A 0.51084 160A → 171A -0.10611 160A → 175A 0.17457 150B → 160B -0.27895 151B → 161B -0.22000 152B → 160B -0.26929 156B → 160B -0.14068 157B → 160B -0.16516 157B → 162B -0.11815 159B → 171B -0.10794	1.542
17	3.6640	338.38	0.0624	150A → 161A -0.16086 151A → 161A 0.10361 156A → 161A -0.18129 157A → 161A 0.15556 160A → 164A 0.17987 160A → 165A 0.29158 160A → 168A 0.13064 160A → 169A 0.10334 149B → 160B -0.25896 150B → 161B 0.33407 151B → 160B 0.43336 153B → 161B 0.11277 154B → 160B -0.26780 155B → 160B -0.19957 156B → 161B 0.16777 159B → 162B 0.18611 159B → 163B 0.10235	1.641

18	3.7084	334.34	0.0035	152A → 161A -0.21362 154A → 161A -0.11934 159A → 164A 0.13242 160A → 166A 0.33039 160A → 167A 0.49826 149B → 161B -0.15327 150B → 160B 0.35628 151B → 161B 0.19862 153B → 160B 0.21341 154B → 161B -0.12329 157B → 160B -0.23907 159B → 165B -0.10957	1.527
19	3.7758	328.37	0.1459	156A → 161A -0.14647 157A → 161A 0.54947 159A → 162A 0.19361 160A → 164A 0.17196 160A → 165A -0.19479 160A → 168A -0.25329 160A → 169A 0.49419 160A → 172A -0.18888 151B → 160B -0.18988 159B → 162B 0.12460	1.287
20	3.8185	324.69	0.0174	149A → 161A 0.12668 155A → 161A -0.19096 158A → 161A 0.13252 159A → 161A 0.23728 160A → 166A 0.17920 149B → 161B -0.11529 151B → 161B -0.18930 155B → 161B -0.26707 156B → 160B -0.34104 157B → 160B 0.17567 159B → 161B 0.66604 159B → 171B -0.12361	1.485
21	3.8972	318.13	0.5940	150A → 161A -0.10467 156A → 161A 0.25698 157A → 161A -0.14411 158A → 162A 0.37266 159A → 162A -0.31600 160A → 164A 0.19253 160A → 165A 0.14190 160A → 168A -0.27412 160A → 169A 0.25436 149B → 160B -0.13610 151B → 160B 0.11103 154B → 160B -0.14966 155B → 160B 0.19319 155B → 162B 0.10093 157B → 161B -0.12727 158B → 160B 0.14126 158B → 162B -0.30412 159B → 162B -0.20241	1.618

22	3.9453	314.26	0.0014	149A → 161A 0.14762 155A → 161A -0.29023 157A → 162A 0.22970 158A → 161A -0.14847 159A → 164A -0.14525 160A → 166A 0.29357 160A → 167A -0.37475 160A → 170A 0.40677 160A → 171A -0.14648 160A → 175A 0.19290 160A → 178A -0.10611 150B → 160B 0.17386 156B → 162B -0.11955 157B → 160B -0.18377 157B → 162B -0.10375 158B → 161B -0.18385 159B → 161B -0.15203	1.362
23	3.9640	312.78	0.0680	151A → 161A 0.10410 155A → 163A 0.13354 156A → 161A -0.31868 156A → 164A -0.10228 157A → 161A -0.28590 158A → 167A -0.11520 159A → 162A -0.19873 160A → 168A 0.33264 160A → 169A 0.28888 160A → 172A -0.19084 149B → 160B 0.19025 155B → 160B 0.33762 156B → 164B 0.12230	1.717
24	3.9898	310.76	0.0052	149A → 161A 0.12337 151A → 163A 0.12375 153A → 167A -0.11263 153A → 171A -0.11305 154A → 172A -0.10580 155A → 161A -0.16517 155A → 164A -0.15106 155A → 168A -0.11626 156A → 163A 0.12965 157A → 162A 0.12875 158A → 168A 0.14757 159A → 164A -0.12679 160A → 167A 0.26817 160A → 183A -0.19737 149B → 164B 0.13361 152B → 160B 0.12544 152B → 163B -0.14555 153B → 160B -0.10908 153B → 166B -0.11078 153B → 167B 0.10243 153B → 170B 0.10685 154B → 169B 0.10551	2.282

				155B → 164B -0.13826 155B → 169B 0.11809 156B → 160B 0.20935 156B → 163B -0.15087 157B → 160B -0.18852 157B → 162B -0.17322 158B → 161B 0.12523 159B → 164B 0.16121	
25	4.0393	306.95	0.4124	156A → 161A -0.33503 157A → 161A -0.19958 159A → 162A 0.35493 160A → 164A 0.23386 160A → 168A 0.25770 160A → 169A -0.13147 160A → 172A -0.10316 151B → 160B -0.17230 152B → 164B -0.12353 155B → 160B 0.22655 155B → 163B -0.11261 158B → 162B -0.29096 158B → 163B -0.12997 159B → 162B 0.19204	1.747
26	4.0854	303.48	0.0000	149A → 161A -0.10015 152A → 161A -0.13553 155A → 161A 0.23098 157A → 162A -0.12330 160A → 167A 0.15399 160A → 170A 0.73429 160A → 171A -0.10932 160A → 176A 0.10224 160A → 178A -0.18587 150B → 160B -0.10518 153B → 160B -0.15569 157B → 160B 0.18662 158B → 161B 0.25500	1.122
27	4.0976	302.58	0.0058	150A → 161A 0.10349 156A → 161A 0.20515 159A → 171A -0.12124 160A → 165A -0.16013 160A → 168A 0.46951 160A → 169A 0.49056 160A → 172A 0.36059 160A → 173A 0.10919 154B → 160B -0.19461 158B → 162B 0.14597	1.349

28	4.1580	298.18	0.0031	152A → 161A 0.19778 154A → 161A 0.10621 155A → 161A -0.26042 160A → 170A 0.21552 160A → 171A 0.72648 160A → 178A -0.12564 153B → 160B 0.23285 156B → 160B 0.11928 158B → 161B 0.13313	1.244
29	4.1653	297.66	0.0029	152A → 161A -0.17556 155A → 161A 0.38206 156A → 162A 0.12046 157A → 162A -0.10124 159A → 161A -0.11597 160A → 170A 0.13011 160A → 171A 0.41590 156B → 160B -0.37069 156B → 162B -0.22409 158B → 161B -0.39341 158B → 169B 0.10267	1.544
30	4.1676	297.49	0.1987	150A → 161A 0.11407 151A → 161A -0.10282 152A → 162A -0.10657 153A → 161A 0.10926 157A → 161A -0.27306 159A → 162A 0.36080 160A → 165A -0.14702 160A → 168A -0.30400 160A → 172A 0.41208 151B → 160B 0.17425 154B → 160B -0.20291 155B → 163B 0.10881 156B → 164B 0.11774 158B → 162B -0.31391 159B → 162B 0.22678	1.383

Table S23. 30 CAM-B3LYP TDDFT transitions of **RC** at the CAM-B3LYP ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	0.8214	1509.50	0.4772	158A → 162A 0.10042 160A → 161A 0.98863 159B → 160B 0.10171 160A → 161A 0.17687	0.816

2	1.7628	703.33	0.0000	159A → 161A 0.34748 160A → 162A 0.84991 157B → 160B 0.16937 158B → 161B -0.11421 159B → 161B -0.21299	1.256
3	2.1004	590.28	0.1535	157A → 161A 0.22286 160A → 161A -0.10983 157B → 161B -0.27513 158B → 160B -0.11823 158B → 162B -0.16452 159B → 160B 0.85986	1.248
4	2.3156	535.43	0.0004	157A → 162A 0.12546 159A → 161A 0.53875 160A → 162A -0.42668 160A → 163A -0.25992 156B → 160B -0.10711 157B → 160B 0.40629 159B → 161B -0.40435	1.875
5	2.5442	487.32	0.4002	157A → 161A 0.14125 159A → 163A -0.10572 160A → 164A -0.17861 152B → 161B 0.16305 156B → 161B -0.14419 157B → 161B -0.17178 158B → 160B 0.83526 159B → 162B 0.10078 159B → 163B 0.14171	1.234
6	2.6670	464.88	0.0001	158A → 161A -0.52392 159A → 161A 0.27270 160A → 162A -0.14007 160A → 163A 0.63673 152B → 160B 0.10673 156B → 160B -0.16268 158B → 161B 0.22874	1.665
7	2.8135	440.67	0.0366	157A → 161A -0.36523 158A → 162A -0.18990 159A → 162A -0.28925 160A → 164A 0.31939 160A → 165A -0.13031 160A → 168A -0.15219 148B → 160B -0.10865 151B → 160B -0.15128 155B → 160B -0.22277 157B → 161B 0.22734 158B → 160B 0.17670 158B → 162B 0.18644 159B → 160B 0.31486 159B → 162B 0.38124	2.014

8	2.9947	414.02	0.0031	158A → 161A 0.59008 160A → 162A -0.16756 160A → 163A 0.57103 160A → 166A 0.19470 152B → 160B -0.15051 155B → 161B 0.10755 156B → 160B 0.12733 158B → 161B -0.23441	1.724
9	3.0870	401.64	0.0531	149A → 161A -0.14834 155A → 161A 0.15493 159A → 161A 0.61152 160A → 163A -0.17289 160A → 167A -0.11999 155B → 161B 0.16614 156B → 160B 0.24320 157B → 160B -0.50005 158B → 161B -0.10850 159B → 161B 0.32765	1.148
10	3.1019	399.70	0.0489	150A → 161A 0.18321 158A → 162A -0.18350 159A → 166A -0.10294 160A → 164A 0.56845 160A → 165A 0.27127 160A → 169A -0.10577 160A → 172A 0.22178 149B → 160B 0.21065 150B → 161B -0.15184 152B → 161B -0.12334 155B → 160B 0.32316 156B → 161B 0.12197 157B → 161B -0.17442 158B → 160B 0.12202 158B → 162B 0.22753 159B → 162B -0.14475	1.505
11	3.2323	383.58	0.1657	150A → 161A 0.10167 158A → 163A 0.10916 159A → 162A -0.16011 159A → 163A -0.21812 160A → 164A -0.22867 160A → 165A 0.36878 160A → 172A 0.14108 149B → 162B -0.10440 150B → 161B -0.12390 151B → 160B -0.17345 155B → 163B -0.10059 158B → 160B -0.18131 158B → 162B -0.10615 159B → 162B 0.50325 159B → 163B 0.21831	2.111

12	3.2357	383.18	0.0006	149A → 161A -0.14511 152A → 161A 0.12968 158A → 161A -0.27423 158A → 165A -0.11792 159A → 165A -0.15633 160A → 163A -0.11310 160A → 166A 0.60783 160A → 170A -0.11978 160A → 171A 0.12747 149B → 161B 0.13527 150B → 160B -0.21909 151B → 161B -0.12742 152B → 160B -0.13500 153B → 160B -0.12878 155B → 161B 0.11861 156B → 160B 0.11217 157B → 160B 0.13962	1.616
13	3.2995	375.76	0.0085	153A → 172A -0.10416 154A → 171A -0.11765 155A → 163A 0.11482 156A → 161A 0.12847 156A → 164A -0.11298 157A → 164A -0.11908 158A → 162A 0.18154 158A → 163A -0.15087 159A → 166A -0.11315 160A → 164A 0.10500 160A → 165A 0.41791 160A → 168A 0.24172 151B → 160B -0.14104 154B → 160B 0.14754 155B → 160B -0.28791 155B → 163B 0.11728 156B → 161B -0.21271 156B → 164B 0.12335 158B → 162B -0.17489 158B → 163B 0.14861 159B → 162B 0.11797 159B → 163B -0.10952	1.965
14	3.3767	367.18	0.0026	158A → 161A -0.24038 160A → 163A 0.18039 160A → 166A -0.20321 149B → 161B -0.13984 150B → 160B 0.23165 151B → 161B 0.10006 156B → 160B 0.47971 157B → 160B 0.38687 157B → 162B 0.12867 158B → 161B -0.41187 158B → 164B -0.10380 159B → 161B 0.23554	1.188

15	3.4000	364.66	0.2508	157A → 161A -0.20053 158A → 162A -0.12165 159A → 162A 0.21636 159A → 163A 0.14146 159A → 167A -0.12476 160A → 164A -0.26650 160A → 165A 0.44929 160A → 168A -0.19206 160A → 169A 0.22756 151B → 160B -0.16863 151B → 162B 0.10065 157B → 161B 0.11103 158B → 160B 0.13764 159B → 160B 0.17507 159B → 162B -0.31434 159B → 163B -0.18508	1.814
16	3.4065	363.96	0.0007	148A → 161A 0.10085 151A → 163A -0.10640 153A → 166A -0.10381 153A → 167A 0.11847 153A → 171A 0.13365 154A → 165A -0.10071 154A → 169A 0.10141 154A → 172A 0.12805 155A → 164A 0.15193 155A → 168A 0.12408 156A → 163A -0.11972 158A → 161A -0.31528 158A → 164A -0.14654 159A → 168A 0.12279 160A → 163A -0.12697 160A → 167A 0.40190 160A → 175A 0.11025 149B → 164B -0.10201 152B → 160B -0.22632 153B → 166B 0.12058 153B → 167B -0.10903 153B → 170B -0.11830 154B → 165B -0.10687 154B → 169B -0.11632 155B → 164B 0.15325 156B → 163B 0.14350 157B → 163B 0.11001 158B → 161B -0.16980 158B → 164B 0.10066	2.062

17	3.5497	349.28	0.0090	151A → 161A 0.13589 156A → 161A -0.25284 158A → 162A -0.18358 160A → 165A 0.39889 160A → 169A 0.13926 149B → 160B -0.19313 150B → 161B 0.29269 151B → 160B 0.38970 154B → 160B -0.22598 155B → 160B -0.10421 156B → 161B 0.20436 158B → 160B -0.12935 158B → 162B 0.20183 159B → 162B 0.12640	1.821
18	3.5737	346.94	0.0001	152A → 161A -0.21884 157A → 162A -0.16202 158A → 161A 0.10282 158A → 165A -0.10260 159A → 164A 0.13249 160A → 163A -0.10232 160A → 166A 0.51268 160A → 170A -0.11675 160A → 175A -0.15173 149B → 161B -0.13321 150B → 160B 0.39213 151B → 161B 0.25428 152B → 160B 0.16125 153B → 160B 0.16624 154B → 161B -0.13162 156B → 160B 0.10206 159B → 165B -0.10449 159B → 171B 0.10159	1.628

19	3.6774	337.16	0.0682	150A → 161A -0.17664 151A → 164A 0.10654 153A → 172A 0.10702 154A → 171A 0.13132 155A → 163A -0.12758 156A → 161A 0.20046 158A → 162A 0.14415 160A → 164A 0.41325 160A → 165A 0.20879 160A → 168A 0.16955 160A → 169A -0.14536 148B → 160B 0.14997 149B → 160B -0.21845 150B → 161B 0.15006 151B → 160B 0.12795 152B → 161B 0.15479 152B → 164B -0.10435 154B → 160B -0.12533 154B → 170B 0.11756 155B → 160B -0.17983 155B → 163B -0.10600 158B → 162B -0.14985	1.898
20	3.6937	335.67	0.0183	149A → 161A 0.17030 155A → 161A -0.16681 158A → 168A 0.10980 159A → 161A 0.15754 159A → 169A -0.11519 160A → 166A 0.24104 160A → 167A 0.41462 160A → 183A -0.14321 147B → 160B 0.12720 149B → 161B -0.14733 151B → 161B -0.10415 155B → 161B -0.21205 156B → 160B -0.20372 157B → 162B -0.14354 159B → 161B 0.43926 159B → 171B -0.11946	1.685
21	3.6951	335.54	0.1416	156A → 161A -0.13917 157A → 161A 0.51214 159A → 162A 0.16838 160A → 164A 0.35705 160A → 165A -0.12502 160A → 168A -0.27880 160A → 169A 0.40569 160A → 172A -0.16068 151B → 160B -0.13841 158B → 162B -0.15509 159B → 160B -0.13496 159B → 162B 0.13214	1.364

22	3.7830	327.74	0.0000	159A → 161A 0.12850 160A → 167A -0.47899 160A → 183A 0.11256 151B → 161B -0.15314 155B → 161B -0.15802 156B → 160B -0.21784 157B → 160B 0.39159 157B → 162B 0.10385 159B → 161B 0.52266	1.465
23	3.7996	326.31	0.5176	157A → 161A 0.33601 158A → 162A -0.30513 159A → 162A 0.41381 160A → 165A -0.14225 160A → 168A 0.20304 160A → 169A -0.33391 160A → 172A 0.14619 151B → 160B -0.14361 155B → 160B -0.29725 155B → 162B -0.10872 157B → 161B 0.17642 158B → 160B -0.12457 158B → 162B 0.24084 159B → 162B 0.11592	1.479
24	3.8632	320.94	0.0024	149A → 161A -0.12627 155A → 161A 0.21649 157A → 162A -0.16929 158A → 161A 0.19708 158A → 165A -0.10403 159A → 161A 0.11332 159A → 164A 0.12971 160A → 166A -0.29386 160A → 167A 0.43283 160A → 170A -0.21789 160A → 175A -0.17274 150B → 160B -0.18795 151B → 161B -0.12046 156B → 162B 0.18359 157B → 160B 0.25553 157B → 163B -0.10211 158B → 161B 0.22463 158B → 164B -0.11552 159B → 161B 0.17415	1.434

25	3.9561	313.40	0.2067	151A → 161A 0.10618 156A → 161A -0.42493 157A → 161A -0.29826 159A → 162A 0.23455 160A → 164A 0.12438 160A → 168A 0.49895 160A → 169A 0.10455 160A → 172A -0.15829 151B → 160B -0.11671 155B → 160B 0.32828 158B → 162B -0.16067 159B → 162B 0.25488	1.270
26	4.0359	307.20	0.0466	156A → 161A 0.29038 157A → 161A 0.12325 159A → 162A -0.13068 159A → 171A -0.10991 160A → 165A -0.13227 160A → 168A 0.48777 160A → 169A 0.55810 160A → 172A 0.10250 158B → 162B 0.27515 159B → 162B -0.12978	1.295
27	4.0484	306.25	0.0006	155A → 161A -0.11037 160A → 166A 0.15426 160A → 170A 0.68985 160A → 171A -0.22197 160A → 175A 0.12956 160A → 176A 0.10200 160A → 178A -0.16887 153B → 160B -0.10126 156B → 160B 0.20975 156B → 162B 0.16640 157B → 160B 0.11956 158B → 161B 0.29656	1.216
28	4.0770	304.11	0.0095	149A → 161A -0.15015 151A → 162A -0.11585 152A → 161A -0.22035 154A → 161A -0.10646 155A → 161A 0.57494 156A → 162A 0.20833 157A → 162A -0.22609 158A → 164A -0.12951 159A → 164A 0.12790 160A → 170A 0.31035 153B → 160B -0.10097 156B → 160B -0.22355 156B → 162B -0.18233 157B → 160B 0.13131 157B → 162B 0.11092	1.971

29	4.1006	302.36	0.1895	150A → 161A 0.16812 151A → 161A -0.11713 152A → 162A -0.15254 156A → 161A 0.12818 157A → 161A -0.25700 158A → 163A -0.10788 159A → 162A 0.37914 159A → 175A -0.10296 160A → 165A -0.19061 160A → 168A -0.18646 160A → 169A 0.13500 160A → 172A 0.42406 148B → 160B -0.10275 149B → 160B -0.10431 151B → 160B 0.14972 154B → 160B -0.27609 158B → 162B -0.23855 159B → 162B 0.21886	1.267
30	4.1348	299.86	0.0020	150A → 162A -0.13445 152A → 161A 0.23813 154A → 161A 0.13377 158A → 169A 0.12013 160A → 166A -0.12544 160A → 167A 0.14077 160A → 170A 0.10308 160A → 171A 0.54686 160A → 175A 0.28852 160A → 177A -0.15735 150B → 160B 0.18608 151B → 161B 0.11776 152B → 160B 0.16407 153B → 160B 0.22411 157B → 162B 0.12237 158B → 161B 0.28622	1.268

D. PBE0

Table S24. 30 CIS calculated transitions of **RC** at the PBE0 ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$<S^2>$
1	1.0783	1149.79	0.5235	160A → 161A 0.96025 158B → 160B 0.15668 159B → 160B -0.12909	0.801
2	1.7198	720.94	0.0000	159A → 161A -0.11941 160A → 162A 0.96393 159B → 161B 0.10843	0.875
3	1.9750	627.77	0.2042	157A → 161A -0.15825 160A → 161A 0.10597 160A → 164A 0.10194 157B → 161B 0.11500 158B → 160B 0.13016 159B → 160B 0.93616	0.925
4	2.1938	565.16	0.0000	159A → 161A 0.70506 160A → 162A 0.16943 160A → 163A 0.18303 157B → 160B -0.42221 159B → 161B -0.44347	2.177
5	2.4349	509.20	0.5778	157A → 161A 0.15377 159A → 162A -0.11732 160A → 161A -0.14210 160A → 164A 0.13141 157B → 161B -0.12303 158B → 160B 0.90788 159B → 162B -0.11604	0.962
6	2.4559	504.84	0.0000	158A → 161A -0.17006 159A → 161A -0.29557 160A → 163A 0.88026 157B → 160B -0.15587 158B → 161B 0.14749	1.062
7	2.7025	458.77	0.0034	158A → 161A 0.82123 159A → 161A 0.15042 160A → 163A 0.30865 160A → 166A 0.10766 152B → 160B -0.12920 156B → 160B 0.15377 157B → 160B 0.13513 158B → 161B -0.29883	2.090

8	2.7783	446.26	0.0283	157A → 161A 0.41538 158A → 162A 0.14807 159A → 162A -0.20959 160A → 164A 0.56939 160A → 165A -0.20959 160A → 168A -0.11020 151B → 160B 0.11196 155B → 160B -0.15683 157B → 161B -0.28789 158B → 160B -0.19150 158B → 162B -0.18816 159B → 162B 0.29902	1.778
9	2.8279	438.44	0.0177	155A → 161A -0.11175 158A → 161A -0.20834 159A → 161A 0.26158 160A → 163A 0.18783 160A → 166A 0.11990 160A → 167A -0.15591 157B → 160B 0.81139 159B → 161B -0.27639	1.241
10	2.8638	432.93	0.0768	157A → 161A -0.22743 160A → 164A 0.65916 160A → 165A 0.45794 160A → 171A -0.13634 149B → 160B 0.14505 155B → 160B 0.31972 157B → 161B 0.20278 159B → 160B -0.12731 159B → 162B -0.11206	1.146
11	2.9211	424.45	0.0197	159A → 161A 0.42041 160A → 166A 0.31063 160A → 167A -0.14645 160A → 172A -0.10888 156B → 160B -0.28713 158B → 161B 0.27583 159B → 161B 0.69139	0.972
12	2.9487	420.47	0.0016	155A → 161A 0.11182 158A → 161A -0.14553 159A → 161A -0.17264 160A → 166A 0.86005 150B → 160B -0.10750 152B → 160B -0.14493 155B → 161B -0.10051 156B → 160B 0.14062 158B → 161B -0.13083 159B → 161B -0.15013	0.935

13	2.9493	420.38	0.0501	157A → 161A 0.20200 159A → 162A -0.10602 160A → 164A -0.27268 160A → 165A 0.80072 160A → 169A -0.10998 151B→ 160B 0.14209 155B → 160B -0.14089 157B → 161B -0.19107 159B → 160B 0.11040 159B → 162B 0.27857	1.166
14	3.1052	399.29	0.2557	157A → 161A -0.28428 159A → 162A -0.47674 159A → 163A -0.20568 160A → 165A -0.14444 160A → 168A -0.13510 160A → 169A 0.13692 155B → 160B 0.20515 157B → 161B 0.14173 158B → 160B 0.10814 159B → 160B -0.12154 159B → 162B 0.59949 159B → 163B -0.19377	2.418
15	3.1528	393.25	0.0282	150A → 161A -0.12864 156A → 161A 0.17995 157A → 161A 0.30526 158A → 162A 0.24945 160A → 164A -0.26047 160A → 168A -0.42562 160A → 171A -0.14217 152B → 161B 0.12825 155B → 160B 0.54931 156B → 161B -0.13029 158B → 162B -0.23903 159B → 162B -0.17761	1.476
16	3.2084	386.44	0.0062	158A → 161A -0.12517 150B → 160B 0.12776 151B → 161B 0.16101 152B → 160B 0.12290 155B → 161B -0.10011 156B → 160B 0.82331 157B → 160B 0.12207 157B → 162B 0.13161 158B → 161B 0.13667 159B → 161B 0.32392	1.115

17	3.2141	385.74	0.0002	158A → 161A 0.25277 160A → 166A 0.10821 160A → 167A 0.80663 160A → 170A -0.11832 152B → 160B 0.18063 153B → 160B -0.10231 156B → 160B -0.11818 157B → 160B 0.14095 158B → 161B 0.30866	0.909
18	3.2769	378.36	0.0011	157A → 161A 0.46533 160A → 168A 0.44582 160A → 169A 0.65151 160A → 171A -0.16627 151B → 160B -0.18410 157B → 161B 0.14702	0.993
19	3.3104	374.52	0.0101	150A → 161A -0.10915 151A → 161A -0.14163 156A → 161A -0.26341 158A → 162A -0.19936 160A → 165A -0.15792 150B → 161B 0.21603 151B → 160B 0.48334 154B → 160B 0.49593 155B → 160B 0.21134 156B → 161B 0.19835 158B → 162B 0.23788 159B → 162B -0.14252 159B → 163B 0.11083	1.554
20	3.3439	370.77	0.0000	149A → 161A 0.12346 152A → 161A -0.21405 154A → 161A 0.12119 155A → 161A -0.20992 160A → 166A 0.27780 160A → 172A -0.19364 149B → 161B 0.15071 150B → 160B 0.47463 151B → 161B 0.18998 152B → 160B 0.26939 153B → 160B 0.48028 155B → 161B 0.17803 157B → 160B -0.10649 158B → 161B -0.20527	1.396
21	3.4100	363.59	0.0017	156A → 161A 0.19166 157A → 161A 0.15688 158A → 162A -0.15591 159A → 162A -0.13010 160A → 168A 0.54885 160A → 169A -0.44654 149B → 160B -0.12594 154B → 160B -0.22381	1.148

				155B → 160B 0.47008 158B → 162B 0.21218	
22	3.4248	362.02	0.0122	157A → 162A -0.14495 158A → 161A 0.27736 159A → 161A -0.17876 160A → 167A -0.36606 160A → 170A -0.33020 152B → 160B -0.10945 153B → 160B 0.25322 156B → 162B 0.11231 158B → 161B 0.64486 159B → 161B -0.19164	0.980
23	3.4539	358.97	0.0380	150A → 161A 0.11736 156A → 161A -0.15148 157A → 161A 0.20119 158A → 162A -0.39722 160A → 164A 0.10497 160A → 165A 0.10380 160A → 168A -0.42472 160A → 169A 0.21629 160A → 171A 0.15071 149B → 160B -0.21217 154B → 160B -0.39709 158B → 162B 0.44030	1.672
24	3.4865	355.61	0.0010	160A → 166A 0.12067 160A → 170A 0.86431 160A → 172A 0.12023 152B → 160B -0.15019 158B → 161B 0.33741	0.958
25	3.5055	353.69	0.0407	156A → 161A 0.47202 159A → 162A 0.11108 160A → 169A 0.14884 160A → 171A 0.48277 151B → 160B -0.20501 154B → 160B 0.56529 155B → 160B 0.13790 159B → 162B 0.15623	1.224
26	3.5231	351.92	0.0083	152A → 161A 0.17324 154A → 161A -0.10269 160A → 167A 0.23459 160A → 172A 0.11306 150B → 160B -0.28620 152B → 160B -0.24698 153B → 160B 0.79450	0.998

27	3.5344	350.79	0.0783	156A → 161A 0.49999 157A → 161A 0.24579 158A → 162A -0.10474 159A → 162A 0.35227 160A → 165A -0.11859 160A → 168A -0.11071 160A → 169A -0.14319 160A → 171A -0.38006 149B→ 160B 0.18988 151B → 160B 0.17939 155B → 160B -0.25958 157B → 161B 0.24596 158B → 162B 0.16983 159B → 162B 0.25504	1.222
28	3.5846	345.88	0.1437	150A → 161A -0.14346 156A → 161A 0.21376 157A → 161A -0.16633 158A → 162A 0.15366 159A → 162A 0.13435 160A → 168A 0.13660 160A → 169A 0.33278 160A → 171A 0.43636 150B → 161B 0.10798 151B → 160B 0.53655 154B → 160B -0.39802 157B → 161B -0.12597	0.980
29	3.6133	343.14	0.0045	149A → 161A -0.12064 152A → 161A -0.15049 154A → 161A 0.13467 155A → 161A 0.72897 157A → 162A -0.22471 159A → 164A 0.11955 160A → 170A 0.12874 160A → 172A -0.23812 150B → 160B 0.21559 151B → 161B 0.10943 152B → 160B -0.15760 155B → 161B -0.16628 156B → 160B -0.23329 157B → 160B 0.10061 157B → 162B 0.15233	1.986
30	3.6541	339.30	1.4889	156A → 161A -0.26236 157A → 161A -0.14711 159A → 162A 0.59685 160A → 169A 0.11376 160A → 171A -0.23876 149B → 160B -0.18667 151B → 160B -0.13523 155B → 160B 0.23522 157B → 161B -0.37952 159B → 162B 0.38227	1.004

Table S25. 30 PBE0 TDDFT transitions of **RC** at the PBE0 ground state doublet geometry.

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions	$\langle S^2 \rangle$
1	0.9225	1343.97	0.3653	160A → 161A 0.97472 158B → 160B 0.12027 159B → 160B -0.13772	0.783
2	1.6451	753.66	0.0000	159A → 161A -0.21360 160A → 162A 0.93565 157B → 160B 0.12244 159B → 161B 0.16606	0.984
3	1.8638	665.22	0.1567	157A → 161A -0.17452 160A → 161A 0.13452 157B → 161B 0.15310 158B → 160B 0.12765 158B → 162B 0.10811 159B → 160B 0.92720	0.969
4	2.0849	594.68	0.0001	158A → 161A -0.10449 159A → 161A 0.66451 160A → 162A 0.30255 160A → 163A 0.17684 156B → 160B 0.10026 157B → 160B -0.40252 158B → 161B 0.10888 159B → 161B -0.43539	2.103
5	2.3326	531.52	0.4054	157A → 161A 0.15246 160A → 161A -0.12441 160A → 164A 0.15561 152B → 161B 0.11121 157B → 161B -0.13756 158B → 160B 0.90009 159B → 163B 0.10185	1.009
6	2.4025	516.06	0.0000	158A → 161A -0.18897 159A → 161A -0.30802 160A → 163A 0.86831 157B → 160B -0.16560 158B → 161B 0.13812	1.097
7	2.6573	466.58	0.0040	158A → 161A 0.79801 159A → 161A 0.22391 160A → 163A 0.33837 160A → 166A 0.11097 152B → 160B -0.12720 156B → 160B 0.12794 157B → 160B 0.11921 158B → 161B -0.28254	2.036

8	2.6582	466.43	0.0289	157A → 161A 0.45456 158A → 162A 0.20872 159A → 162A -0.22967 160A → 164A 0.38146 160A → 165A -0.18221 160A → 168A -0.11979 151B → 160B 0.10543 155B → 160B -0.20421 157B → 161B -0.31903 158B → 160B -0.18538 158B → 162B -0.21743 159B → 160B 0.20900 159B → 162B 0.31824	2.059
9	2.7688	447.80	0.0276	155A → 161A -0.13052 158A → 161A -0.23424 159A → 161A 0.40999 160A → 163A 0.20775 160A → 167A -0.15447 160A → 172A -0.10161 155B → 161B 0.10342 156B → 160B -0.14966 157B → 160B 0.76078 158B → 161B 0.13057	1.180
10	2.7985	443.04	0.0668	157A → 161A -0.15472 160A → 164A 0.74610 160A → 165A 0.35626 160A → 171A -0.15299 149B → 160B 0.14999 150B → 161B 0.10071 155B → 160B 0.29423 157B → 161B 0.15746 158B → 160B -0.11453 159B → 160B -0.10944	1.074
11	2.8635	432.98	0.0067	159A → 161A 0.35638 160A → 166A -0.12054 152B → 160B 0.10016 156B → 160B -0.29997 157B → 160B -0.30801 158B → 161B 0.25662 159B → 161B 0.73370	1.020
12	2.8999	427.55	0.0004	158A → 161A -0.12833 160A → 166A 0.86771 160A → 170A -0.10239 150B → 160B -0.16382 152B → 160B -0.13123 153B → 160B -0.11042 155B → 161B -0.10287 159B → 161B 0.18528	1.038

13	2.9129	425.64	0.0230	157A → 161A 0.12874 159A → 162A -0.10464 160A → 164A -0.31779 160A → 165A 0.81838 151B → 160B 0.13230 157B → 161B -0.12960 159B → 162B 0.27637	1.118
14	3.0259	409.75	0.1885	157A → 161A -0.19992 159A → 162A -0.39524 159A → 163A -0.24108 160A → 164A -0.10102 160A → 165A -0.25207 160A → 168A -0.18395 160A → 169A 0.17047 160A → 171A -0.11535 155B → 160B 0.31549 157B → 161B 0.12511 158B → 160B 0.15021 159B → 162B 0.49701 159B → 163B -0.23612	2.153
15	3.0808	402.44	0.0531	150A → 161A -0.11599 156A → 161A 0.15517 157A → 161A 0.31397 158A → 162A 0.25518 159A → 162A 0.12900 160A → 164A -0.23672 160A → 168A -0.33566 160A → 171A -0.10649 152B → 161B 0.11338 155B → 160B 0.45147 156B → 161B -0.13358 158B → 162B -0.24160 159B → 160B 0.12007 159B → 162B -0.39367	1.813
16	3.1443	394.31	0.0039	158A → 164A -0.10154 160A → 167A 0.57442 160A → 170A -0.12710 151B → 161B 0.12410 152B → 160B 0.18258 153B → 160B -0.11087 156B → 160B 0.50468 157B → 160B 0.16965 157B → 162B 0.11655 157B → 163B 0.10475 158B → 161B 0.22523 159B → 161B 0.22554	1.265

17	3.1644	391.82	0.0022	155A → 161A 0.11856 158A → 161A -0.30717 159A → 161A 0.10347 160A → 166A -0.14188 160A → 167A -0.47290 150B → 160B 0.10797 152B → 160B -0.12041 155B → 161B -0.10498 156B → 160B 0.61028 158B → 161B -0.23074 159B → 161B 0.31274	0.975
18	3.2194	385.11	0.0005	150A → 161A -0.12599 156A → 161A -0.11005 157A → 161A -0.20635 158A → 162A -0.23673 160A → 165A -0.15350 160A → 168A -0.38763 160A → 169A -0.39003 150B → 161B 0.15742 151B → 160B 0.46077 154B → 160B 0.24233 155B → 160B 0.13287 156B → 161B 0.11925 157B → 161B -0.10671 158B → 160B -0.14588 158B → 162B 0.24006 159B → 163B 0.10364	1.382
19	3.2441	382.19	0.0102	151A → 161A -0.12949 156A → 161A -0.19498 157A → 161A 0.40165 158A → 162A -0.10706 159A → 162A -0.11178 160A → 164A -0.10966 160A → 165A -0.13047 160A → 168A 0.29018 160A → 169A 0.47475 160A → 171A -0.18089 148B → 160B -0.10145 149B → 160B 0.15032 150B → 161B 0.15982 151B → 160B 0.23313 154B → 160B 0.30784 155B → 160B 0.18862 156B → 161B 0.13541 158B → 162B 0.15576	1.340

20	3.2631	379.96	0.0001	149A → 161A 0.11316 152A → 161A -0.24217 154A → 161A 0.13046 155A → 161A -0.17279 160A → 166A 0.37988 160A → 172A -0.19769 149B → 161B 0.15304 150B → 160B 0.46840 151B → 161B 0.21792 152B → 160B 0.29449 153B → 160B 0.37463 154B → 161B 0.11220 155B → 161B 0.16964	1.450
21	3.3522	369.86	0.0092	157A → 162A -0.12158 158A → 161A 0.29643 159A → 161A -0.16964 160A → 167A -0.44182 160A → 170A -0.12438 156B → 160B 0.17664 156B → 162B 0.12367 158B → 161B 0.72070 159B → 161B -0.12392	1.062
22	3.3655	368.40	0.0202	156A → 161A 0.12445 157A → 161A 0.37738 158A → 162A -0.32879 159A → 162A -0.12181 160A → 164A 0.11933 160A → 168A 0.17751 160A → 169A -0.18395 160A → 171A 0.10755 149B → 160B -0.20819 150B → 161B -0.10212 151B → 160B -0.11194 154B → 160B -0.36724 155B → 160B 0.38386 155B → 162B 0.11113 158B → 160B -0.10946 158B → 162B 0.38691 159B → 162B 0.11921	1.713
23	3.3994	364.73	0.0231	150A → 161A -0.10873 156A → 161A 0.18312 157A → 161A -0.10639 158A → 162A 0.18927 160A → 164A -0.11129 160A → 165A -0.11053 160A → 168A 0.58055 160A → 169A -0.48371 149B → 160B 0.11700 154B → 160B 0.15170 155B → 160B 0.31155 157B → 161B -0.11800 158B → 162B -0.20259	1.218

24	3.4516	359.21	0.0028	155A → 164A -0.11036 160A → 167A 0.35042 160A → 170A 0.55004 160A → 172A 0.13904 152B → 160B -0.24436 153B → 160B 0.31307 155B → 164B 0.10602 156B → 163B -0.10856 157B → 160B 0.10979 158B → 161B 0.21788	1.474
25	3.4727	357.02	0.0576	151A → 161A 0.10233 156A → 161A 0.53796 159A → 162A 0.18035 160A → 168A -0.23155 160A → 169A 0.20302 160A → 171A 0.32148 151B → 160B -0.16076 154B → 160B 0.44534 159B → 162B 0.26674	1.451
26	3.4750	356.79	0.0040	155A → 161A -0.17207 160A → 166A 0.10004 160A → 167A -0.10749 160A → 170A 0.66126 152B → 160B 0.13330 153B → 160B -0.55226 157B → 162B -0.11539 158B → 161B 0.11706	1.123
27	3.4970	354.55	0.2465	150A → 161A -0.10917 156A → 161A 0.36975 157A → 161A 0.16070 159A → 162A 0.50830 160A → 165A -0.14422 160A → 171A -0.38832 149B → 160B 0.11705 151B → 160B 0.25733 154B → 160B -0.20966 155B → 160B -0.23808 159B → 162B 0.30078	1.132

28	3.5169	352.54	0.2293	153A → 161A 0.11482 153A → 171A -0.10013 154A → 170A -0.11047 155A → 163A 0.13152 156A → 164A 0.10032 157A → 161A -0.19349 158A → 163A -0.12125 159A → 162A 0.24610 160A → 164A 0.14288 160A → 168A 0.31878 160A → 169A 0.23789 160A → 171A 0.29279 149B → 160B -0.24185 151B → 160B 0.19445 154B → 160B 0.20221 155B → 160B 0.15418 155B → 163B 0.13839 156B → 164B -0.13118 157B → 161B -0.26566 158B → 163B -0.13088	1.607
29	3.5396	350.27	0.0002	149A → 161A 0.12088 152A → 161A 0.16436 154A → 161A -0.14728 155A → 161A -0.34451 156A → 163A 0.12328 157A → 162A 0.15341 159A → 164A -0.14513 160A → 170A 0.12324 160A → 172A 0.13875 150B → 160B -0.25114 151B → 161B -0.10598 153B → 160B 0.55995 155B → 164B -0.10434 156B → 160B 0.13555 156B → 163B 0.11920 157B → 162B -0.14033 159B → 164B 0.12537	1.779
30	3.5485	349.40	0.1254	150A → 161A 0.11376 157A → 161A 0.21687 159A → 163A -0.21203 160A → 164A 0.11905 160A → 169A -0.33237 160A → 171A -0.22637 151B → 160B -0.27336 154B → 160B 0.56847 155B → 160B -0.15808 157B → 161B 0.22100 159B → 162B -0.15948 159B → 163B -0.19691	1.304

VII. Optimized Structures

A. DC Ground and Excited State Structures

Ground State (S_0) Structure of **DC** (D3-B3LYP)**:**

2 1

N	2.02448700	-1.80213300	0.98114700
C	-3.05765000	-1.77573400	-1.05030300
H	-2.31502500	-2.50959700	-1.32152400
C	1.00407800	-0.94057100	0.55310500
N	-2.02449900	1.80211400	0.98118300
C	-6.01549400	1.12771400	-0.15038700
C	1.34018600	0.41263700	0.23011400
C	5.01162800	-0.16736800	-0.46379600
C	-3.66609800	0.35571500	-0.03400800
C	-1.55650100	-3.43231300	1.16058100
H	-2.06197700	-2.81630800	1.89805000
C	0.32274000	1.38847000	0.36961700
C	0.61953800	2.84549800	0.29397700
C	3.32528500	-1.55492600	0.67205800
C	7.33445100	-0.91632400	-0.58261900
H	8.09693700	-1.64861100	-0.33482000
C	-0.61953700	-2.84551400	0.29407500
C	-4.34900100	2.49184100	1.00981800
H	-4.10765200	3.40071600	1.54195400
C	0.24190400	5.01107600	-0.73703700
H	-0.26667800	5.62030200	-1.47764200
C	-2.68935100	-0.64898700	-0.26146500
C	2.68933800	0.64899200	-0.26145200
C	5.36283000	0.99258700	-1.20952600
C	-0.04079600	3.64631900	-0.65140300
H	-0.76410900	3.19646900	-1.32476900
C	5.63937900	-2.28174200	0.60439800
H	6.39767100	-3.02135000	0.84273800
C	1.72287700	-2.86148100	1.97764000
H	2.45299400	-2.78598200	2.78337100
H	1.75305900	-3.85362500	1.52701200
H	0.73954700	-2.68154300	2.39694100
C	4.34126800	1.93316600	-1.51463200
H	4.58490700	2.79337200	-2.13095400
C	-3.32529700	1.55491200	0.67209100
C	-0.32275200	-1.38847900	0.36963000
C	3.66608700	-0.35571000	-0.03401000
C	7.67229900	0.22217800	-1.32414800
H	8.69530600	0.36758600	-1.65388900

C	1.83063700	4.79678900	1.07922000
H	2.55265100	5.24232000	1.75643800
C	0.04075100	-3.64637000	-0.65130800
H	0.76400600	-3.19653900	-1.32474800
C	6.69949700	1.16479600	-1.63635200
H	6.95824500	2.04812700	-2.21216200
C	1.17689700	5.58892300	0.12776600
H	1.39392500	6.65063500	0.06291700
C	-5.63939100	2.28173100	0.60444700
H	-6.39768300	3.02133200	0.84280700
C	-5.01163700	0.16738900	-0.46380800
C	1.55659000	3.43231800	1.16037400
H	2.06211300	2.81633700	1.89783100
C	-6.69950100	-1.16473200	-1.63642100
H	-6.95824600	-2.04804300	-2.21226300
C	-5.36283700	-0.99254000	-1.20957900
C	-1.17684400	-5.58896100	0.12805000
H	-1.39385400	-6.65068000	0.06327000
C	-1.83052400	-4.79679400	1.07951700
H	-2.55247500	-5.24230800	1.75681400
C	-1.34020100	-0.41264500	0.23012100
C	4.34898800	-2.49186500	1.00975900
H	4.10763800	-3.40075600	1.54186800
C	-1.72290500	2.86142300	1.97772400
H	-0.73958300	2.68146700	2.39703700
H	-2.45303500	2.78588900	2.78343900
H	-1.75308100	3.85358500	1.52713700
C	-4.34127300	-1.93310700	-1.51471300
H	-4.58490800	-2.79328800	-2.13107200
C	-0.24192800	-5.01113700	-0.73685300
H	0.26661300	-5.62039000	-1.47746400
C	-7.67230300	-0.22212300	-1.32419200
H	-8.69530800	-0.36751700	-1.65394400
C	-7.33445900	0.91635400	-0.58262300
H	-8.09694400	1.64863500	-0.33480500
C	6.01548500	-1.12770000	-0.15039800
C	-1.00409100	0.94056300	0.55311700
C	3.05764100	1.77577300	-1.05023900
H	2.31501600	2.50964900	-1.32143000

Dipole: 2.241000 Debyes
Energy: -1880.421374 Hartees

Ground State (S_0) Structure of **DC** (B3LYP)**:**

2 1

N	2.02328100	-1.80160000	0.98456200
C	-3.06377800	-1.75744300	-1.07151800
H	-2.32269400	-2.48998600	-1.35099000
C	1.00188700	-0.94396600	0.54721100
N	-2.02321200	1.80170500	0.98437400
C	-6.02068700	1.13341400	-0.12987300
C	1.34069700	0.40948200	0.22115700
C	5.01681800	-0.17880500	-0.46054700
C	-3.66974500	0.36171700	-0.03167600
C	-1.56007900	-3.43758300	1.16584600
H	-2.04895100	-2.82635300	1.91865600
C	0.32684900	1.39139800	0.36139600
C	0.63359800	2.85082900	0.28648500
C	3.32676100	-1.55233500	0.68652600
C	7.34032600	-0.92813800	-0.56334000
H	8.10295800	-1.65562300	-0.30214700
C	-0.63360700	-2.85077900	0.28639400
C	-4.35136300	2.48005300	1.04697300
H	-4.10909400	3.37880500	1.59553000
C	0.29125800	5.01953200	-0.75766200
H	-0.19907700	5.62876600	-1.51065000
C	-2.69249800	-0.63977900	-0.27112300
C	2.69253700	0.63973600	-0.27124500
C	5.36900100	0.96982900	-1.22293900
C	-0.00281100	3.65656300	-0.67269700
H	-0.71387200	3.21375000	-1.36382900
C	5.64343500	-2.27418800	0.64448200
H	6.40213100	-3.00738800	0.90075600
C	1.72118900	-2.85928600	1.98188900
H	2.44078700	-2.77101000	2.79591000
H	1.77219000	-3.85443000	1.53935600
H	0.73047500	-2.68946600	2.38699300
C	4.34752900	1.90639000	-1.54015400
H	4.59155600	2.75808500	-2.16811200
C	-3.32670200	1.55241100	0.68639700
C	-0.32680000	-1.39136700	0.36145800
C	3.66978600	-0.36173700	-0.03171000
C	7.67877000	0.19804500	-1.32306600
H	8.70220200	0.33834000	-1.65383400
C	1.84322600	4.80091700	1.08679400
H	2.55512100	5.24313600	1.77697200
C	0.00291100	-3.65647900	-0.67274400

H	0.71414300	-3.21366400	-1.36369800
C	6.70625700	1.13521300	-1.65135200
H	6.96563600	2.00940200	-2.24070200
C	1.21304700	5.59511400	0.12202500
H	1.43800400	6.65528900	0.05813900
C	-5.64337500	2.27426700	0.64428500
H	-6.40206400	3.00750600	0.90046800
C	-5.01678900	0.17871900	-0.46044800
C	1.55981000	3.43764300	1.16620400
H	2.04855800	2.82639500	1.91908000
C	-6.70626000	-1.13548200	-1.65100400
H	-6.96565700	-2.00976200	-2.24021100
C	-5.36899200	-0.97003300	-1.22265700
C	-1.21326500	-5.59499800	0.12156800
H	-1.43829800	-6.65515000	0.05754600
C	-1.84359100	-4.80082800	1.08626400
H	-2.55567500	-5.24304300	1.77624700
C	-1.34064300	-0.40946000	0.22118700
C	4.35143200	-2.47991800	1.04722400
H	4.10917400	-3.37859100	1.59591700
C	-1.72103000	2.85959000	1.98146200
H	-0.73026200	2.68986100	2.38648100
H	-2.44053400	2.77147000	2.79558200
H	-1.77208800	3.85464500	1.53873400
C	-4.34753300	-1.90665100	-1.53974900
H	-4.59158500	-2.75845300	-2.16755200
C	-0.29125000	-5.01941700	-0.75788200
H	0.19918600	-5.62862700	-1.51082300
C	-7.67876300	-0.19826200	-1.32283500
H	-8.70220500	-0.33860800	-1.65355200
C	-7.34029900	0.92803600	-0.56329100
H	-8.10292300	1.65556100	-0.30218600
C	6.02072600	-1.13345100	-0.12985700
C	-1.00183400	0.94400600	0.54713000
C	3.06379000	1.75726000	-1.07185200
H	2.32270100	2.48974800	-1.35143900

Dipole: 2.27610 debye
Energy: -1880.321788 Hartrees

Ground State (S_0) Structure of **DC** (CAM-B3LYP)**:**

2 1

N	2.01935600	-1.80448400	0.95776700
C	-3.06337900	-1.77535100	-1.02842000
H	-2.32606500	-2.51511600	-1.29474800
C	0.99891200	-0.93799700	0.54024100
N	-2.01935200	1.80450000	0.95774200
C	-5.99677500	1.13243700	-0.14770800
C	1.33512300	0.40797000	0.22830600
C	5.00222400	-0.17186400	-0.45710200
C	-3.65658900	0.35669900	-0.03341200
C	-1.52887300	-3.42969100	1.17717500
H	-2.00934500	-2.82229400	1.93791300
C	0.32376500	1.38232200	0.36253800
C	0.62486300	2.84005500	0.28793400
C	3.31032200	-1.55627800	0.65922900
C	7.30947900	-0.92743300	-0.57285000
H	8.06758500	-1.66417700	-0.32701500
C	-0.62486300	-2.84005100	0.28798000
C	-4.33117400	2.49541300	1.00118600
H	-4.08331900	3.40316600	1.53064100
C	0.28978500	4.99190700	-0.76577200
H	-0.19140500	5.59596200	-1.52766500
C	-2.68984700	-0.64501800	-0.25244800
C	2.68984700	0.64501200	-0.25247200
C	5.35722700	0.98319100	-1.19023200
C	0.00275000	3.63281200	-0.68041600
H	-0.69576200	3.18302500	-1.37914700
C	5.61388900	-2.28771100	0.60246800
H	6.37068800	-3.02814100	0.84091900
C	1.72023900	-2.86155400	1.94777400
H	2.45233200	-2.79099300	2.75064900
H	1.74661900	-3.85350300	1.49817100
H	0.74031100	-2.67942200	2.37153000
C	4.34155400	1.92837600	-1.48773900
H	4.59071700	2.79153300	-2.09684700
C	-3.31031800	1.55629000	0.65921500
C	-0.32376300	-1.38231700	0.36256400
C	3.65658900	-0.35670000	-0.03342100
C	7.65414600	0.20981100	-1.30635900
H	8.67793900	0.35177500	-1.63280900
C	1.80659500	4.78848000	1.09739300
H	2.50522100	5.23664400	1.79602400
C	-0.00275000	-3.63282200	-0.68035700
H	0.69576400	-3.18304600	-1.37909300

C	6.69037200	1.15269800	-1.61304400
H	6.95250900	2.03826000	-2.18287900
C	1.19063900	5.57240600	0.12309000
H	1.41148100	6.63267800	0.05877800
C	-5.61388500	2.28772300	0.60244700
H	-6.37068300	3.02815800	0.84088500
C	-5.00222400	0.17185600	-0.45708600
C	1.52886900	3.42970900	1.17712300
H	2.00934000	2.82232500	1.93787100
C	-6.69037800	-1.15272600	-1.61299900
H	-6.95251700	-2.03829800	-2.18281600
C	-5.35723000	-0.98321200	-1.19019400
C	-1.19064400	-5.57240200	0.12317300
H	-1.41148800	-6.63267500	0.05887500
C	-1.80660100	-4.78846100	1.09746300
H	-2.50523000	-5.23661500	1.79609800
C	-1.33512100	-0.40796800	0.22832000
C	4.33117900	-2.49539500	1.00121400
H	4.08332700	-3.40313800	1.53068700
C	-1.72022700	2.86158900	1.94772800
H	-0.74029600	2.67946300	2.37148000
H	-2.45231500	2.79104300	2.75060900
H	-1.74660900	3.85352900	1.49810600
C	-4.34156000	-1.92840500	-1.48768500
H	-4.59072600	-2.79157400	-2.09677500
C	-0.28978800	-4.99191700	-0.76569500
H	0.19140300	-5.59598400	-1.52757900
C	-7.65414900	-0.20983200	-1.30632900
H	-8.67794400	-0.35180100	-1.63277400
C	-7.30947900	0.92742500	-0.57284200
H	-8.06758300	1.66417400	-0.32701900
C	5.99677700	-1.13243800	-0.14770800
C	-0.99890900	0.93800500	0.54022700
C	3.06337500	1.77533000	-1.02846800
H	2.32605900	2.51508800	-1.29480900

Dipole: 2.3342 debye
Energy: -1879.241705 Hartrees

Ground State (S_0) Structure of **DC** (PBE0)**:**

2 1

N	2.00723600	-1.81010800	0.96031800
C	-3.06270800	-1.75805900	-1.04442700
H	-2.32299000	-2.49562700	-1.32016600
C	0.99668300	-0.94595300	0.53857600
N	-2.00724800	1.81011100	0.96033400
C	-5.99560300	1.14627000	-0.12489700
C	1.33810700	0.40269400	0.22074200
C	5.00108700	-0.18666300	-0.44687900
C	-3.65562000	0.36949000	-0.02965300
C	-1.57343700	-3.41255300	1.15348500
H	-2.06080600	-2.79699300	1.90483600
C	0.33074000	1.38353700	0.35729000
C	0.64262300	2.83381400	0.27985900
C	3.30544300	-1.56379800	0.66999100
C	7.31464700	-0.94129800	-0.54602100
H	8.07277600	-1.67595200	-0.28971600
C	-0.64261500	-2.83380000	0.27993300
C	-4.32014700	2.49922000	1.02232000
H	-4.06987800	3.40521100	1.55717500
C	0.30922200	4.99359500	-0.76509400
H	-0.17980400	5.60505600	-1.51749900
C	-2.68738500	-0.63507300	-0.26078900
C	2.68738300	0.63508300	-0.26078600
C	5.35989800	0.96666800	-1.18914900
C	0.00776500	3.63633300	-0.67660800
H	-0.70866500	3.19332200	-1.36329200
C	5.61128500	-2.29374900	0.62908900
H	6.36630900	-3.03403100	0.87787300
C	1.70064600	-2.87699100	1.92725800
H	2.41656400	-2.80657000	2.74719600
H	1.74769800	-3.86539500	1.46733200
H	0.70814400	-2.71227400	2.33302000
C	4.34658300	1.90794700	-1.50175500
H	4.59780700	2.76553700	-2.11964700
C	-3.30545200	1.56379800	0.67000500
C	-0.33074200	-1.38351700	0.35730300
C	3.65561400	-0.36948400	-0.02965500
C	7.66097700	0.19101600	-1.28630400
H	8.68713200	0.33218700	-1.60909600
C	1.86309500	4.77019600	1.07016100
H	2.58000500	5.21074000	1.75661900
C	-0.00767500	-3.63637500	-0.67643200
H	0.70880800	-3.19340200	-1.36308600

C	6.69612500	1.13327400	-1.60660600
H	6.96117200	2.01501300	-2.18294100
C	1.23527200	5.56302000	0.10803200
H	1.46631800	6.62198200	0.04098200
C	-5.61130000	2.29373200	0.62913000
H	-6.36632800	3.03400500	0.87793000
C	-5.00109400	0.18666300	-0.44686900
C	1.57338900	3.41261500	1.15344100
H	2.06069800	2.79709900	1.90486600
C	-6.69613100	-1.13327300	-1.60659600
H	-6.96117700	-2.01501000	-2.18293600
C	-5.35990300	-0.96666400	-1.18914400
C	-1.23523000	-5.56302100	0.10823400
H	-1.46626400	-6.62198800	0.04123300
C	-1.86313000	-4.77014200	1.07026700
H	-2.58008800	-5.21064700	1.75670000
C	-1.33810800	-0.40267700	0.22073500
C	4.32013200	-2.49923500	1.02228200
H	4.06985900	-3.40523400	1.55712200
C	-1.70068300	2.87694700	1.92733500
H	-0.70818600	2.71222300	2.33310400
H	-2.41661100	2.80647100	2.74725800
H	-1.74774300	3.86537700	1.46746400
C	-4.34658600	-1.90793900	-1.50175500
H	-4.59780900	-2.76552900	-2.11964900
C	-0.30911500	-4.99364500	-0.76485600
H	0.17997200	-5.60515000	-1.51718400
C	-7.66098600	-0.19102200	-1.28628300
H	-8.68714200	-0.33219700	-1.60907100
C	-7.31465900	0.94128700	-0.54599100
H	-8.07279100	1.67593400	-0.28967600
C	5.99559300	-1.14627800	-0.12492200
C	-0.99668800	0.94597200	0.53856700
C	3.06270600	1.75806900	-1.04442500
H	2.32298800	2.49563900	-1.32016000

Dipole: 2.1900 debye
Energy: -1878.136758 Hartrees

TDDFT Optimized Emissive Excited State (S_2) Structure of **DC** (D3-B3LYP, from excited state 2 in Table S6):

2 1

N	1.99874000	-1.82708600	0.99474200
C	-3.03015000	-1.71891500	-1.10759900
H	-2.27594500	-2.43144400	-1.40659000
C	0.98777800	-0.97783000	0.54871500
N	-1.99869100	1.82717000	0.99460500
C	-5.99213600	1.18678900	-0.19301800
C	1.34243200	0.38080600	0.20395400
C	4.98543900	-0.22744700	-0.50663000
C	-3.64621600	0.41914700	-0.07155700
C	-1.72510200	-3.34107400	1.16045000
H	-2.25526400	-2.66940900	1.82824500
C	0.33867400	1.39442900	0.37574300
C	0.69678400	2.83466800	0.33953200
C	3.31264500	-1.60220300	0.65014600
C	7.31271400	-0.96858700	-0.63405400
H	8.07787300	-1.70031500	-0.39251800
C	-0.69678300	-2.83463100	0.33946400
C	-4.32615100	2.54307300	0.97167700
H	-4.08399200	3.44872900	1.51033200
C	0.35338600	5.06378800	-0.56299000
H	-0.17242800	5.72996500	-1.23963500
C	-2.66270500	-0.59155500	-0.30473400
C	2.66272500	0.59151900	-0.30483500
C	5.33497500	0.94017400	-1.25843400
C	0.01244900	3.71265200	-0.52004100
H	-0.77501300	3.32878400	-1.16102700
C	5.62290300	-2.33904100	0.56038400
H	6.38082500	-3.07875500	0.79803100
C	1.69894700	-2.86583800	2.00480500
H	2.43359100	-2.78297300	2.80690400
H	1.72369000	-3.86740000	1.57273500
H	0.71578700	-2.67884700	2.42483200
C	4.31643800	1.88231100	-1.56767300
H	4.56028200	2.73937900	-2.18752600
C	-3.31260200	1.60226600	0.65004200
C	-0.33863900	-1.39440200	0.37578600
C	3.64624200	-0.41916000	-0.07158100
C	7.64654400	0.17227100	-1.37662500
H	8.66931600	0.31782100	-1.70753200
C	2.05297400	4.69504800	1.12575100
H	2.84026000	5.07482200	1.76915700
C	-0.01238600	-3.71259100	-0.52008400

H	0.77518200	-3.32872000	-1.16093700
C	6.67395000	1.11383900	-1.68915800
H	6.92971600	1.99699800	-2.26612900
C	1.37200200	5.55961300	0.26150900
H	1.63278000	6.61277800	0.22867900
C	-5.62285700	2.33911100	0.56021700
H	-6.38077000	3.07885900	0.79778800
C	-4.98542300	0.22738500	-0.50655300
C	1.72494300	3.34112000	1.16071800
H	2.25503100	2.66944600	1.82856100
C	-6.67396500	-1.11404400	-1.68887200
H	-6.92974900	-1.99727800	-2.26572200
C	-5.33498100	-0.94033100	-1.25820100
C	-1.37213900	-5.55953200	0.26116000
H	-1.63296800	-6.61268200	0.22822600
C	-2.05319700	-4.69498200	1.12535100
H	-2.84060300	-5.07475500	1.76861300
C	-1.34239400	-0.38078800	0.20397800
C	4.32620400	-2.54296300	0.97188300
H	4.08405600	-3.44855800	1.51064600
C	-1.69883900	2.86606100	2.00450600
H	-0.71564300	2.67913300	2.42448200
H	-2.43342200	2.78330200	2.80667100
H	-1.72361600	3.86756300	1.57229900
C	-4.31645800	-1.88252200	-1.56732900
H	-4.56032500	-2.73968100	-2.18704700
C	-0.35338400	-5.06370700	-0.56316500
H	0.17249200	-5.72986800	-1.23977800
C	-7.64654700	-0.17242900	-1.37644100
H	-8.66932700	-0.31801600	-1.70730800
C	-7.31269800	0.96852100	-0.63402200
H	-8.07784800	1.70028200	-0.39256100
C	5.99216200	-1.18680800	-0.19299700
C	-0.98774000	0.97786400	0.54865800
C	3.03014200	1.71875700	-1.10788900
H	2.27592300	2.43122100	-1.40699700

Dipole: 2.042700 Debyes
Energy: -1880.341951 Hartrees

DFT Optimized Triplet Excited State (T_1) Structure of **DC** (D3-B3LYP):

2 3

N	1.98278100	-1.76425500	1.00026100
C	-3.09134300	-1.73640600	-1.12970900
H	-2.35111600	-2.45437900	-1.45089000
C	1.00598200	-0.93652400	0.52266100
N	-1.98277800	1.76427800	1.00023400
C	-6.03480800	1.13407300	-0.03970300
C	1.35967400	0.41232700	0.15349600
C	5.03990600	-0.17870600	-0.40637700
C	-3.68506100	0.35890700	-0.00929500
C	-1.62625000	-3.42043400	1.03740600
H	-2.17722000	-2.80281200	1.73964000
C	0.34669000	1.38241800	0.31513200
C	0.63557200	2.83508100	0.22883800
C	3.33301000	-1.52380900	0.71616400
C	7.37878100	-0.92514000	-0.44346900
H	8.13319500	-1.65087700	-0.15570500
C	-0.63556600	-2.83507700	0.22887400
C	-4.32266400	2.46097100	1.08533300
H	-4.06477900	3.35817700	1.62973800
C	0.19690900	5.00269200	-0.77441100
H	-0.35371900	5.61255800	-1.48355700
C	-2.70346200	-0.63814400	-0.31298700
C	2.70345600	0.63813800	-0.31301800
C	5.40880600	0.96140200	-1.17943200
C	-0.08224200	3.63887400	-0.67355800
H	-0.84431300	3.19241200	-1.30500500
C	5.64065000	-2.26528200	0.71695700
H	6.38566900	-3.00257700	0.99818200
C	1.66522900	-2.83749700	1.97406800
H	2.35340700	-2.73330200	2.81315900
H	1.76180200	-3.82493100	1.52230200
H	0.65582800	-2.70019800	2.34343900
C	4.38981900	1.88775700	-1.55285500
H	4.65227300	2.72729800	-2.18923400
C	-3.33300900	1.52382600	0.71615000
C	-0.34669100	-1.38241100	0.31515400
C	3.68505800	-0.35890700	-0.00931000
C	7.72680200	0.18850200	-1.19715600
H	8.75724400	0.33504300	-1.50322200
C	1.89085900	4.78463700	0.94484600
H	2.64948700	5.22988600	1.58078800
C	0.08223700	-3.63886900	-0.67353400
H	0.84429400	-3.19240500	-1.30499600

C	6.75248300	1.12421100	-1.56795400
H	7.02823900	1.98932600	-2.16323100
C	1.18065300	5.57898800	0.03531000
H	1.39242100	6.64103600	-0.03896400
C	-5.64064900	2.26529900	0.71694100
H	-6.38566700	3.00260000	0.99815400
C	-5.03991300	0.17869700	-0.40634900
C	1.62626900	3.42043500	1.03735600
H	2.17724600	2.80281200	1.73958400
C	-6.75249700	-1.12424700	-1.56788500
H	-7.02825800	-1.98937600	-2.16314000
C	-5.40881800	-0.96142900	-1.17937400
C	-1.18063200	-5.57898900	0.03536400
H	-1.39239500	-6.64103800	-0.03890200
C	-1.89083000	-4.78463900	0.94490600
H	-2.64944500	-5.22989000	1.58086100
C	-1.35967700	-0.41232400	0.15351200
C	4.32266600	-2.46094600	1.08536100
H	4.06478400	-3.35814100	1.62978700
C	-1.66521800	2.83754700	1.97400700
H	-0.65581500	2.70025900	2.34337300
H	-2.35339000	2.73337700	2.81310700
H	-1.76179500	3.82496800	1.52221400
C	-4.38983400	-1.88779400	-1.55278100
H	-4.65229200	-2.72735100	-2.18913800
C	-0.19690600	-5.00268900	-0.77437600
H	0.35371300	-5.61255500	-1.48352900
C	-7.72681400	-0.18852900	-1.19710300
H	-8.75725700	-0.33507600	-1.50316000
C	-7.37878800	0.92513000	-0.44344400
H	-8.13319900	1.65087500	-0.15569200
C	6.03480400	-1.13407300	-0.03971400
C	-1.00598200	0.93653500	0.52264900
C	3.09133100	1.73637900	-1.12977000
H	2.35110100	2.45434400	-1.45096300

Dipole: 3.323300 Debyes
Energy: -1880.369071 Hartrees

B. RC Ground and Excited State Structures

Ground State (D_0) Structure of **RC** (D3-B3LYP):

1 2

N	2.02953900	-1.79242000	0.97810800
C	-3.06141500	-1.79938200	-1.02943200
H	-2.31809000	-2.53955000	-1.28362400
C	1.00853000	-0.94141300	0.54527000
N	-2.02954100	1.79240400	0.97812000
C	-6.02396100	1.13663600	-0.20856900
C	1.34760400	0.41822700	0.22525800
C	5.01796000	-0.16407900	-0.49290900
C	-3.67312800	0.35875900	-0.05340000
C	-1.53721400	-3.42778700	1.21142500
H	-2.04015300	-2.79865900	1.93981000
C	0.31623700	1.38955400	0.37352900
C	0.61131800	2.85057700	0.32678000
C	3.34175000	-1.55867600	0.63407100
C	7.34543600	-0.91562500	-0.65203300
H	8.10748800	-1.65670600	-0.42872800
C	-0.61132200	-2.85060600	0.32686600
C	-4.35600600	2.51084300	0.93080300
H	-4.11023500	3.42923500	1.44657000
C	0.23782800	5.03964200	-0.66429400
H	-0.26787200	5.66135700	-1.39700300
C	-2.68572900	-0.65610000	-0.25799300
C	2.68571500	0.65609500	-0.25798900
C	5.36765900	1.01328400	-1.21981100
C	-0.03902200	3.67153100	-0.60824900
H	-0.75667900	3.23283500	-1.29524600
C	5.65079800	-2.30355900	0.52009700
H	6.40634300	-3.05313400	0.73574200
C	1.74520800	-2.82489900	1.99652400
H	2.50432400	-2.75435600	2.77720700
H	1.73985100	-3.82962100	1.56991800
H	0.77792700	-2.62180500	2.44521200
C	4.33843100	1.96528000	-1.49748500
H	4.58085200	2.83672500	-2.09893900
C	-3.34175300	1.55866500	0.63409100
C	-0.31624900	-1.38957900	0.37354600
C	3.67312000	-0.35875900	-0.05340400
C	7.67388100	0.23493100	-1.36688800
H	8.69403900	0.38905300	-1.70406300
C	1.81109000	4.79432900	1.15846900
H	2.52760800	5.22740500	1.85005500

C	0.03891500	-3.67157600	-0.60822100
H	0.75647700	-3.23288700	-1.29532100
C	6.69629500	1.19136200	-1.65120600
H	6.95426400	2.08663500	-2.20942800
C	1.16395300	5.60505600	0.21818300
H	1.37878000	6.66854200	0.17561600
C	-5.65079700	2.30356400	0.52012300
H	-6.40633800	3.05313900	0.73577800
C	-5.01796700	0.16409900	-0.49292100
C	1.53734000	3.42776500	1.21119800
H	2.04036600	2.79864700	1.93953200
C	-6.69630000	-1.19129900	-1.65127000
H	-6.95427100	-2.08655400	-2.20951900
C	-5.36766700	-1.01324100	-1.21985800
C	-1.16392500	-5.60509700	0.21841500
H	-1.37874200	-6.66858800	0.17590300
C	-1.81094900	-4.79435600	1.15876700
H	-2.52737000	-5.22742600	1.85045900
C	-1.34762000	-0.41825000	0.22527400
C	4.35600700	-2.51085300	0.93077100
H	4.11023900	-3.42925400	1.44652200
C	-1.74520300	2.82488500	1.99653400
H	-0.77792600	2.62178500	2.44522500
H	-2.50432200	2.75435300	2.77721400
H	-1.73983500	3.82960500	1.56992100
C	-4.33844100	-1.96523000	-1.49755700
H	-4.58086000	-2.83665100	-2.09904700
C	-0.23792300	-5.03969200	-0.66419600
H	0.26769200	-5.66141800	-1.39695400
C	-7.67388400	-0.23487000	-1.36693400
H	-8.69403900	-0.38897600	-1.70412300
C	-7.34543700	0.91566600	-0.65204800
H	-8.10748400	1.65674800	-0.42873200
C	6.02395900	-1.13661400	-0.20856900
C	-1.00853900	0.94139000	0.54528100
C	3.06140200	1.79941000	-1.02937600
H	2.31807500	2.53958700	-1.28353900

Dipole: 2.947900 Debyes
Energy: -1880.580730 Hartrees

Ground State (D_0) Structure of **RC** (B3LYP):

1 2

N	2.02899200	-1.79192800	0.98270200

C	-3.06528300	-1.78144500	-1.05091500
H	-2.32283400	-2.52008500	-1.31262300
C	1.00671500	-0.94459200	0.54235100
N	-2.02905000	1.79198800	0.98271500
C	-6.02927400	1.14152900	-0.19101600
C	1.34788500	0.41529800	0.21877500
C	5.02230200	-0.17464800	-0.49160700
C	-3.67640800	0.36459200	-0.05171400
C	-1.53777000	-3.43464500	1.22096300
H	-2.02259000	-2.81132600	1.96676600
C	0.31998200	1.39260500	0.36885500
C	0.62446200	2.85614800	0.32258300
C	3.34403200	-1.55625900	0.64852600
C	7.35085600	-0.92598400	-0.63700600
H	8.11371600	-1.66230000	-0.40099800
C	-0.62441600	-2.85612900	0.32257000
C	-4.36033100	2.49978100	0.96640400
H	-4.11497100	3.40921200	1.49792100
C	0.28708200	5.04740800	-0.68447000
H	-0.19936200	5.66831700	-1.43094400
C	-2.68797100	-0.64706900	-0.26724700
C	2.68791600	0.64704300	-0.26739800
C	5.37165900	0.99185300	-1.23580800
C	-0.00065700	3.68101300	-0.62778700
H	-0.70450900	3.24857700	-1.33306800
C	5.65626400	-2.29592400	0.55762000
H	6.41277400	-3.03951000	0.79009300
C	1.74458100	-2.82154100	2.00359600
H	2.49695700	-2.73999600	2.78984800
H	1.75459300	-3.82986100	1.58529900
H	0.77182100	-2.62448400	2.44237800
C	4.34175000	1.93958800	-1.52482500
H	4.58342900	2.80296000	-2.13817800
C	-3.34408500	1.55634600	0.64838000
C	-0.32005100	-1.39256000	0.36893900
C	3.67636600	-0.36459200	-0.05175500
C	7.67852200	0.21289300	-1.37053800
H	8.69868800	0.36236900	-1.70989200
C	1.82069500	4.79990300	1.16875600
H	2.52563600	5.23050200	1.87384000
C	0.00069500	-3.68083500	-0.62791000
H	0.70452700	-3.24829100	-1.33314300
C	6.70040300	1.16378800	-1.67015800
H	6.95802300	2.05038500	-2.24224900
C	1.19847800	5.61158800	0.21335300
H	1.42110800	6.67351800	0.17068300

C	-5.65623000	2.29622800	0.55707300
H	-6.41266200	3.03999500	0.78918000
C	-5.02234600	0.17466400	-0.49159100
C	1.53789600	3.43452700	1.22096200
H	2.02280700	2.81109300	1.96659100
C	-6.70051700	-1.16405200	-1.66975900
H	-6.95814700	-2.05079400	-2.24160800
C	-5.37174500	-0.99203300	-1.23551000
C	-1.19830400	-5.61156900	0.21304400
H	-1.42087900	-6.67350400	0.17027000
C	-1.82050100	-4.80002300	1.16857400
H	-2.52543000	-5.23072000	1.87359800
C	-1.34791500	-0.41530700	0.21891600
C	4.36036600	-2.49948300	0.96691400
H	4.11508100	-3.40875500	1.49868700
C	-1.74458900	2.82145000	2.00370500
H	-0.77205400	2.62392200	2.44288500
H	-2.49728400	2.74026100	2.78967800
H	-1.75397000	3.82980600	1.58547500
C	-4.34186100	-1.93981700	-1.52437200
H	-4.58353900	-2.80329600	-2.13756600
C	-0.28695900	-5.04724900	-0.68474000
H	0.19951900	-5.66803400	-1.43130400
C	-7.67860200	-0.21308200	-1.37033800
H	-8.69880400	-0.36263200	-1.70955800
C	-7.35087400	0.92599700	-0.63713700
H	-8.11371500	1.66239700	-0.40135300
C	6.02925000	-1.14139000	-0.19082200
C	-1.00670400	0.94468200	0.54230000
C	3.06519400	1.78130000	-1.05132100
H	2.32272400	2.51987100	-1.31312400

Dipole: 2.977905 Debyes
Energy: -1880.481220 Hartrees

Ground State (D_0) Structure of **RC** (CAM-B3LYP):

1 2

N	2.01727300	-1.79405100	0.96133600
C	-3.06191000	-1.78923300	-1.02168500
H	-2.32214500	-2.53163800	-1.27675400
C	1.00130000	-0.94418100	0.53409900
N	-2.01711100	1.79424900	0.96100800
C	-6.00250300	1.14490800	-0.19941500
C	1.34400200	0.41155700	0.21788100

C	5.00584700	-0.17610400	-0.48544400
C	-3.66031200	0.36874700	-0.05327800
C	-1.52486800	-3.42181400	1.22234500
H	-2.00404800	-2.79883200	1.97143200
C	0.31968200	1.38575000	0.36615900
C	0.62376500	2.84596500	0.32117900
C	3.32574200	-1.56072200	0.62600900
C	7.32087600	-0.92897400	-0.63492300
H	8.07918900	-1.67223000	-0.40912900
C	-0.62379700	-2.84586900	0.32099300
C	-4.33525600	2.51450500	0.92826000
H	-4.08315900	3.43025500	1.44426500
C	0.29519800	5.02432700	-0.68883300
H	-0.18513000	5.64369300	-1.43939000
C	-2.67890700	-0.64353400	-0.25657800
C	2.67897700	0.64344400	-0.25681200
C	5.35880800	0.99462400	-1.20532300
C	0.00919400	3.66305700	-0.63203600
H	-0.68907800	3.22805800	-1.34058600
C	5.62422500	-2.31051900	0.52678100
H	6.37839500	-3.05952500	0.74610400
C	1.73420100	-2.82625200	1.97058400
H	2.49536100	-2.76238100	2.74823700
H	1.72417000	-3.83003000	1.54372000
H	0.77062700	-2.62093100	2.42411100
C	4.33231100	1.94964500	-1.48380300
H	4.58063500	2.82001700	-2.08323600
C	-3.32563500	1.56087700	0.62572700
C	-0.31961000	-1.38568200	0.36633600
C	3.66038500	-0.36878000	-0.05334600
C	7.65378500	0.21613600	-1.34436000
H	8.67473300	0.36881700	-1.67734100
C	1.80707100	4.78155100	1.17067900
H	2.50594500	5.21357000	1.87969700
C	-0.00904300	-3.66283500	-0.63221200
H	0.68952900	-3.22778200	-1.34043400
C	6.68160200	1.17086700	-1.62989400
H	6.94264700	2.06600300	-2.18573100
C	1.19518300	5.58765300	0.21201500
H	1.41785600	6.64880100	0.16924000
C	-5.62410900	2.31069100	0.52629800
H	-6.37825300	3.05978400	0.74541600
C	-5.00579400	0.17595100	-0.48526300
C	1.52436700	3.42186200	1.22303100
H	2.00333000	2.79880000	1.97219000
C	-6.68162100	-1.17137400	-1.62921500

H	-6.94270400	-2.06668300	-2.18475600
C	-5.35879900	-0.99500800	-1.20477400
C	-1.19558700	-5.58744600	0.21101900
H	-1.41839100	-6.64855500	0.16794200
C	-1.80773800	-4.78145300	1.16960800
H	-2.50694900	-5.21351900	1.87826500
C	-1.34388000	-0.41153100	0.21794800
C	4.33541900	-2.51423200	0.92886100
H	4.08336200	-3.42981900	1.44517100
C	-1.73388500	2.82674300	1.96988400
H	-0.77023400	2.62154000	2.42332800
H	-2.49493200	2.76316000	2.74767500
H	-1.72387000	3.83039700	1.54271400
C	-4.33233100	-1.95013100	-1.48300700
H	-4.58070000	-2.82070500	-2.08212700
C	-0.29520900	-5.02405400	-0.68939300
H	0.18529700	-5.64332800	-1.43991200
C	-7.65378600	-0.21653700	-1.34392800
H	-8.67475100	-0.36932100	-1.67681000
C	-7.32084100	0.92879200	-0.63487600
H	-8.07913600	1.67212800	-0.40928400
C	6.00257500	-1.14495600	-0.19934100
C	-1.00117200	0.94427600	0.53392400
C	3.06193200	1.78890500	-1.02234400
H	2.32214900	2.53120200	-1.27764400

Dipole: 2.921710 Debyes
Energy: -1879.399921 Hartrees

Ground State (D_0) Structure of **RC** (PBE0):

1 2

N	2.00895800	-1.80147100	0.95766500
C	-3.06921100	-1.77380300	-1.02961600
H	-2.32818100	-2.51448900	-1.29577800
C	1.00041500	-0.94772500	0.52902100
N	-2.00895700	1.80149700	0.95764100
C	-6.00794000	1.15389900	-0.16095500
C	1.34594700	0.40707800	0.21337400
C	5.01109200	-0.18486700	-0.46265000
C	-3.66416700	0.37468000	-0.04215400
C	-1.55666800	-3.41458600	1.18405100
H	-2.04380000	-2.79105500	1.92922000
C	0.32615400	1.38433800	0.35654300
C	0.63548100	2.83850200	0.29856300

C	3.32110700	-1.56837700	0.64012300
C	7.33185200	-0.93826000	-0.58642000
H	8.08970700	-1.67960200	-0.34811200
C	-0.63547600	-2.83847400	0.29860000
C	-4.32640000	2.51731900	0.95771000
H	-4.07064600	3.43332200	1.47476900
C	0.30187600	5.01554800	-0.71961600
H	-0.18672000	5.63435400	-1.46678800
C	-2.68534600	-0.63802200	-0.25891200
C	2.68535500	0.63802700	-0.25892900
C	5.37003600	0.98382500	-1.18894400
C	0.00796300	3.65483500	-0.65110000
H	-0.70390100	3.21806300	-1.34680800
C	5.62431500	-2.31337400	0.56701500
H	6.37634400	-3.06230000	0.79875600
C	1.71277700	-2.84669900	1.94125200
H	2.45797400	-2.78860500	2.73711100
H	1.71881800	-3.84567800	1.49892100
H	0.73658700	-2.65556200	2.37749000
C	4.34869600	1.93291500	-1.48484900
H	4.60005800	2.79939700	-2.09060600
C	-3.32110600	1.56838900	0.64011300
C	-0.32614400	-1.38431100	0.35655900
C	3.66417100	-0.37467900	-0.04216100
C	7.67041700	0.20453900	-1.30187200
H	8.69540100	0.35537100	-1.62658000
C	1.84467600	4.77419300	1.11956600
H	2.55722200	5.20730100	1.81579600
C	-0.00786000	-3.65484900	-0.65096200
H	0.70408600	-3.21810900	-1.34660600
C	6.70047300	1.15754300	-1.60377200
H	6.96594200	2.04965900	-2.16436300
C	1.22055300	5.57912100	0.16501800
H	1.44823000	6.63982800	0.11287800
C	-5.62432300	2.31336000	0.56702300
H	-6.37635800	3.06228000	0.79876700
C	-5.01109200	0.18484700	-0.46262100
C	1.55656900	3.41465700	1.18409500
H	2.04362200	2.79115900	1.92934300
C	-6.70047300	-1.15760000	-1.60369800
H	-6.96594100	-2.04973000	-2.16426800
C	-5.37003300	-0.98386400	-1.18888700
C	-1.22055900	-5.57909200	0.16509400
H	-1.44824000	-6.63980000	0.11296800
C	-1.84478200	-4.77412200	1.11954100
H	-2.55741000	-5.20719700	1.81570600

C	-1.34593700	-0.40705300	0.21337000
C	4.32639300	-2.51731600	0.95771500
H	4.07063200	-3.43331400	1.47478000
C	-1.71278600	2.84672900	1.94122900
H	-0.73658100	2.65562000	2.37744500
H	-2.45796500	2.78860700	2.73710200
H	-1.71886600	3.84570800	1.49890100
C	-4.34869100	-1.93295900	-1.48477300
H	-4.60005600	-2.79945900	-2.09050200
C	-0.30177700	-5.01556100	-0.71945900
H	0.18689700	-5.63440100	-1.46655200
C	-7.67042100	-0.20459700	-1.30180800
H	-8.69540700	-0.35544300	-1.62650400
C	-7.33185800	0.93821700	-0.58638000
H	-8.08971800	1.67955700	-0.34807600
C	6.00793500	-1.15392300	-0.16097800
C	-1.00041100	0.94775400	0.52900100
C	3.06921800	1.77377900	-1.02967700
H	2.32819000	2.51445800	-1.29586000

Dipole: 2.867500 Debyes
Energy: -1878.298980 Hartrees

TDDFT Optimized Emissive Excited State (D_4) Structure of **RC** (D3-B3LYP, from excited state 5 in Table S17):

1 2

N	2.07673000	-1.76128500	1.04656500
C	-2.94070600	-1.84556400	-1.04122400
H	-2.18925000	-2.60815400	-1.18746600
C	1.01028500	-0.96386400	0.60702900
N	-2.07668300	1.76137400	1.04645000
C	-5.91639400	1.17699500	-0.61254100
C	1.33559700	0.41511800	0.25318300
C	4.89660200	-0.18891100	-0.77616200
C	-3.60754000	0.38192400	-0.21192200
C	-1.66133600	-3.25791700	1.52472900
H	-2.18453000	-2.51140500	2.11491500
C	0.29028400	1.41399600	0.49921800
C	0.64604400	2.85003200	0.64033600
C	3.34429800	-1.56554300	0.52084800
C	7.18896500	-0.95942700	-1.19591100
H	7.96004300	-1.71456600	-1.07291400
C	-0.64604600	-2.84999900	0.64028400
C	-4.36612900	2.52826600	0.70128300

H	-4.16577000	3.43739000	1.25411400
C	0.32630800	5.17597000	-0.00469900
H	-0.19083500	5.91662900	-0.60744600
C	-2.60187800	-0.65534200	-0.30447800
C	2.60189700	0.65532700	-0.30456000
C	5.19247200	1.01401500	-1.49894600
C	-0.01667400	3.82822400	-0.12263500
H	-0.79699500	3.52491400	-0.81439700
C	5.61569800	-2.34071100	0.14240600
H	6.38114700	-3.09950500	0.27321500
C	1.89578800	-2.70773200	2.15693500
H	2.72640600	-2.58823300	2.85680300
H	1.84814800	-3.74494100	1.81538300
H	0.96844400	-2.46804900	2.67283500
C	4.16896800	2.00754200	-1.62277900
H	4.37779400	2.90295200	-2.20046900
C	-3.34425800	1.56560000	0.52075900
C	-0.29025200	-1.41396200	0.49925900
C	3.60756200	-0.38193100	-0.21194200
C	7.45731000	0.20496300	-1.91563800
H	8.43806000	0.35285800	-2.35623300
C	1.99810200	4.60598100	1.64867300
H	2.78007100	4.90359500	2.34099000
C	0.01667200	-3.82816200	-0.12272300
H	0.79704200	-3.52483300	-0.81442300
C	6.47316200	1.18473300	-2.06506600
H	6.68780300	2.09446600	-2.61795700
C	1.33402600	5.57100200	0.88246500
H	1.60075800	6.61950000	0.97406300
C	-5.61565600	2.34075300	0.14226400
H	-6.38109600	3.09956600	0.27300700
C	-4.89659100	0.18885400	-0.77610000
C	1.66125100	3.25793100	1.52488800
H	2.18442600	2.51140200	2.11506700
C	-6.47318300	-1.18491200	-2.06483200
H	-6.68784200	-2.09470100	-2.61762400
C	-5.19248200	-1.01414400	-1.49875600
C	-1.33414300	-5.57096000	0.88218700
H	-1.60091500	-6.61945500	0.97370300
C	-1.99823900	-4.60596400	1.64841000
H	-2.78026600	-4.90359400	2.34065500
C	-1.33556500	-0.41509200	0.25320800
C	4.36618000	-2.52818000	0.70146000
H	4.16583500	-3.43725100	1.25438200
C	-1.89568100	2.70795900	2.15669100
H	-0.96831400	2.46832700	2.67257600

H	-2.72626800	2.58856700	2.85661400
H	-1.84803600	3.74512300	1.81500000
C	-4.16898900	-2.00769600	-1.62249900
H	-4.37783700	-2.90317100	-2.20008200
C	-0.32636100	-5.17590400	-0.00489200
H	0.19079300	-5.91654200	-0.60765600
C	-7.45732200	-0.20511800	-1.91548900
H	-8.43808100	-0.35305200	-2.35605000
C	-7.18895600	0.95934400	-1.19588600
H	-7.96002600	1.71450100	-1.07295200
C	5.91641500	-1.17702800	-0.61252100
C	-1.01025000	0.96390500	0.60698100
C	2.94069900	1.84546400	-1.04145800
H	2.18923400	2.60802500	-1.18778600

Dipole: 2.695000 Debyes
Energy: -1880.507159 Hartrees

DFT optimized Quartet Excited State (Q_1) Structure of **RC** (D3-B3LYP):

1 4

N	1.99510400	-1.77976300	0.95534200
C	-3.12283400	-1.79168500	-1.04681900
H	-2.38969600	-2.53314500	-1.32972700
C	1.01055000	-0.93051200	0.49877800
N	-1.99507900	1.77981000	0.95526500
C	-6.05116700	1.15910700	-0.15319500
C	1.36259000	0.42027600	0.16569100
C	5.06405000	-0.16295400	-0.44274800
C	-3.70959200	0.34269000	-0.02998000
C	-1.55786400	-3.41567600	1.15505000
H	-2.07788800	-2.78696300	1.87118200
C	0.34499200	1.37467200	0.32511500
C	0.62375000	2.83636100	0.28031200
C	3.35262000	-1.55065600	0.62433800
C	7.39919800	-0.94043400	-0.56349500
H	8.14533900	-1.69577300	-0.33561200
C	-0.62375400	-2.83634200	0.28031500
C	-4.31951200	2.52879300	0.88972000
H	-4.04650000	3.46056600	1.36744200
C	0.21296000	5.02371900	-0.69423700
H	-0.30842900	5.64391100	-1.41688000
C	-2.73486100	-0.67533900	-0.28019300
C	2.73487500	0.67532200	-0.28025200
C	5.43979900	1.01674700	-1.15917700

C	-0.05171700	3.65331100	-0.64039600
H	-0.77558700	3.21221800	-1.31880500
C	5.64840200	-2.33172600	0.52100400
H	6.38243100	-3.10029100	0.74190100
C	1.70914100	-2.78928800	1.99258700
H	2.46033600	-2.68318500	2.77811100
H	1.73356300	-3.80437900	1.59142100
H	0.73218900	-2.59745700	2.42463200
C	4.43085600	1.96406500	-1.47260300
H	4.69158200	2.83782900	-2.06233000
C	-3.35259800	1.55068800	0.62428400
C	-0.34497500	-1.37465900	0.32515100
C	3.70960700	-0.34269600	-0.02999800
C	7.75216900	0.21528400	-1.24994500
H	8.78214200	0.36551200	-1.55908400
C	1.81280000	4.78509200	1.10796000
H	2.53151900	5.22308200	1.79385200
C	0.05171700	-3.65328800	-0.64039500
H	0.77562000	-3.21219700	-1.31877000
C	6.79090500	1.18564500	-1.55338400
H	7.07089100	2.08116600	-2.10012200
C	1.14401200	5.59315300	0.17986700
H	1.34596300	6.65922700	0.14141300
C	-5.64838100	2.33175300	0.52092100
H	-6.38240700	3.10033200	0.74177800
C	-5.06403800	0.16292200	-0.44270500
C	1.55780200	3.41570100	1.15510500
H	2.07781100	2.78698700	1.87124700
C	-6.79090400	-1.18574600	-1.55323900
H	-7.07089600	-2.08130100	-2.09991900
C	-5.43979400	-1.01682400	-1.15905700
C	-1.14409000	-5.59311800	0.17978300
H	-1.34606800	-6.65918600	0.14129800
C	-1.81289500	-4.78505900	1.10786600
H	-2.53165400	-5.22304500	1.79371800
C	-1.36257200	-0.42026700	0.16571300
C	4.31953700	-2.52874400	0.88982600
H	4.04652800	-3.46048800	1.36760600
C	-1.70908800	2.78941600	1.99242300
H	-0.73212200	2.59762000	2.42445200
H	-2.46026000	2.68337800	2.77797800
H	-1.73352000	3.80447500	1.59117300
C	-4.43085600	-1.96416400	-1.47243200
H	-4.69159000	-2.83796900	-2.06209600
C	-0.21299300	-5.02368700	-0.69427500
H	0.30840500	-5.64387600	-1.41691500

C	-7.75216600	-0.21536500	-1.24985100
H	-8.78214100	-0.36561300	-1.55897100
C	-7.39918800	0.94039500	-0.56347700
H	-8.14532600	1.69574800	-0.33563300
C	6.05118200	-1.15912100	-0.15318700
C	-1.01053000	0.93053100	0.49874800
C	3.12284000	1.79161500	-1.04696100
H	2.38970000	2.53305300	-1.32991900

Dipole: 3.864800 Debyes
Energy: -1880.516701 Hartrees

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