Subphthalocyanine-radiaannulene scaffold – a multi-electron acceptor and strong chromophore

Henriette Lissau, Cecilie Lindholm Andersen, Freja Eilsø Storm, Marco Santella, Ole Hammerich, Thorsten Hansen, Kurt V. Mikkelsen, and Mogens Brøndsted Nielsen*

Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark. E-mail: mbn@chem.ku.dk

Electronic supporting information

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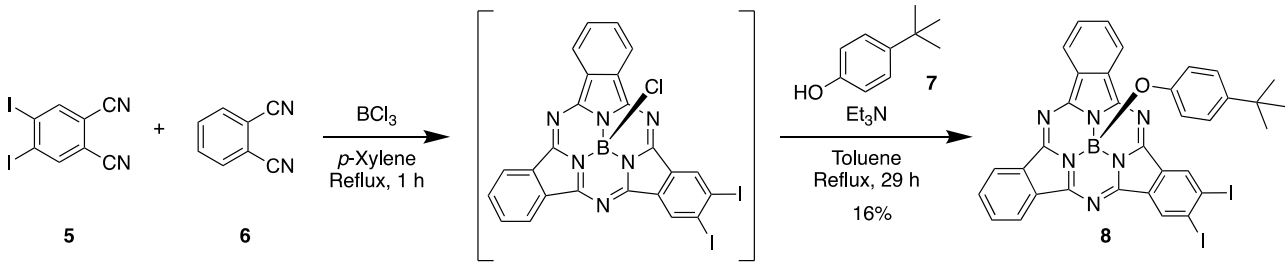
Synthesis

General methods. Dry toluene was obtained from a solvent purification system Pure Solv. Column chromatography was performed on ROCC silica gel ROCC 60 Å (40-63 μm). Thin layer chromatography (TLC) was performed on commercially available precoated plates (silica gel 60 F_{254}) with a fluorescence indicator. The NMR spectra were recorded on a Bruker 500 MHz instrument equipped with a cryoprobe (non-inverse). All the chemical shift values in ^{1}H and ^{13}C NMR spectra are referenced to the residual solvent peak ($CDCl_3$ δ_H = 7.26 ppm, δ_C = 77.16 ppm). In the ^{13}C APT NMR spectra, negative signals correspond to CH and CH_3, while positive signals correspond to C and CH_2. Mass spectra were obtained by the use of a MALDI-FT-ICR instrument equipped with a 7T magnet.

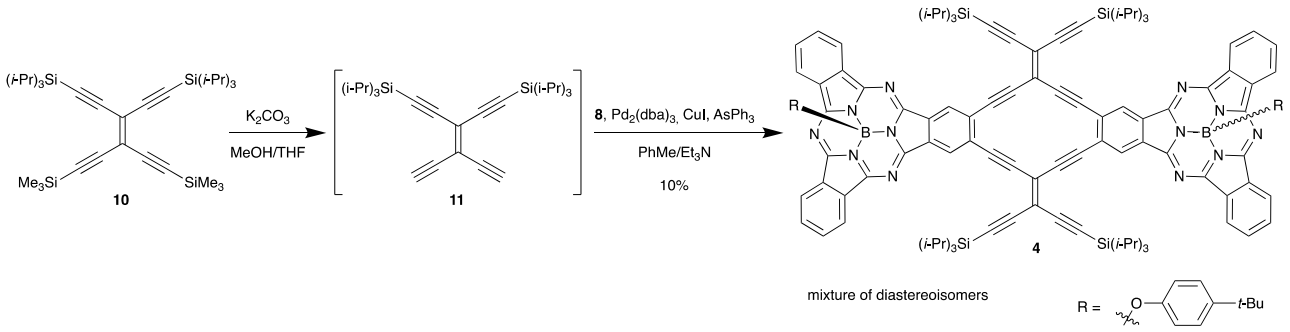
Compound 8



An argon-flushed mixture of 4,5-diiodophthalonitrile **5** (1.84 g, 4.85 mmol) and phthalonitrile **6** (12.5 g, 97.3 mmol) was dissolved in BCl_3 (51 mL, 1 M in *p*-xylene, 51.0 mmol), and the mixture was refluxed for 1 h under an argon atmosphere. A color change to dark purple was observed. The reaction mixture was cooled to rt with a flow of N_2, and then toluene and CH_2Cl_2 were added, and the mixture was concentrated at a rotary evaporator. The purple/blue residue was dried overnight on an oil pump and was then treated with 4-*tert*-butylphenol **7** (20.4 g, 136 mmol), dry toluene (100 mL), and Et_3N (4.7 mL, 33.7 mmol), and the mixture was stirred at reflux for 24 h. Then a new portion of 4-*tert*-butylphenol (10.2 g, 67.9 mmol) was added, and the mixture was heated further at reflux for 5 h. After removal of the solvent *in vacuo*, some excess of the 4-*tert*-butylphenol was sublimed at 100 °C under reduced pressure (using a "cold finger" setup). The residue was purified by flash column chromatography (SiO_2, toluene) several times to separate the four products into three fractions. Isolation of **8** was performed by removal of remaining 4-*tert*-butylphenol by N_2-flow, while the mixture was heated to 100 °C. Subsequently, repeated purification by flash column chromatography

(SiO_2, 70% CH_2Cl_2/toluene) followed by size exclusion chromatography (bio-beads S-X3, CH_2Cl_2), and finally repeated flash column chromatography (SiO_2, 70% CH_2Cl_2/toluene and toluene) gave the product **8** (625 mg, 16%) as a dark pink-purple powder. TLC (toluene): R_f = 0.23; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.37 (s, 2H), 8.87-8.79 (m, 4H), 7.94-7.89 (m, 4H), 6.75 (d, J = 8.6 Hz, 2H), 5.28 (d, J = 8.6 Hz, 2H), 1.08 (s, 9H) ppm; ^{13}C APT NMR (125 MHz, $CDCl_3$): δ 152.86, 151.95, 149.94, 148.70, 143.98, 132.57, 131.36, 131.19, 130.93, 130.44, 130.30, 125.88, 122.55, 122.41, 117.88, 108.76, 33.98, 31.45 ppm; HRMS (MALDI+): m/z = 797.01949 [M+H$^+$], calcd for $C_{34}H_{24}BI_2N_6O^+$: m/z = 797.01885.

Compound 4

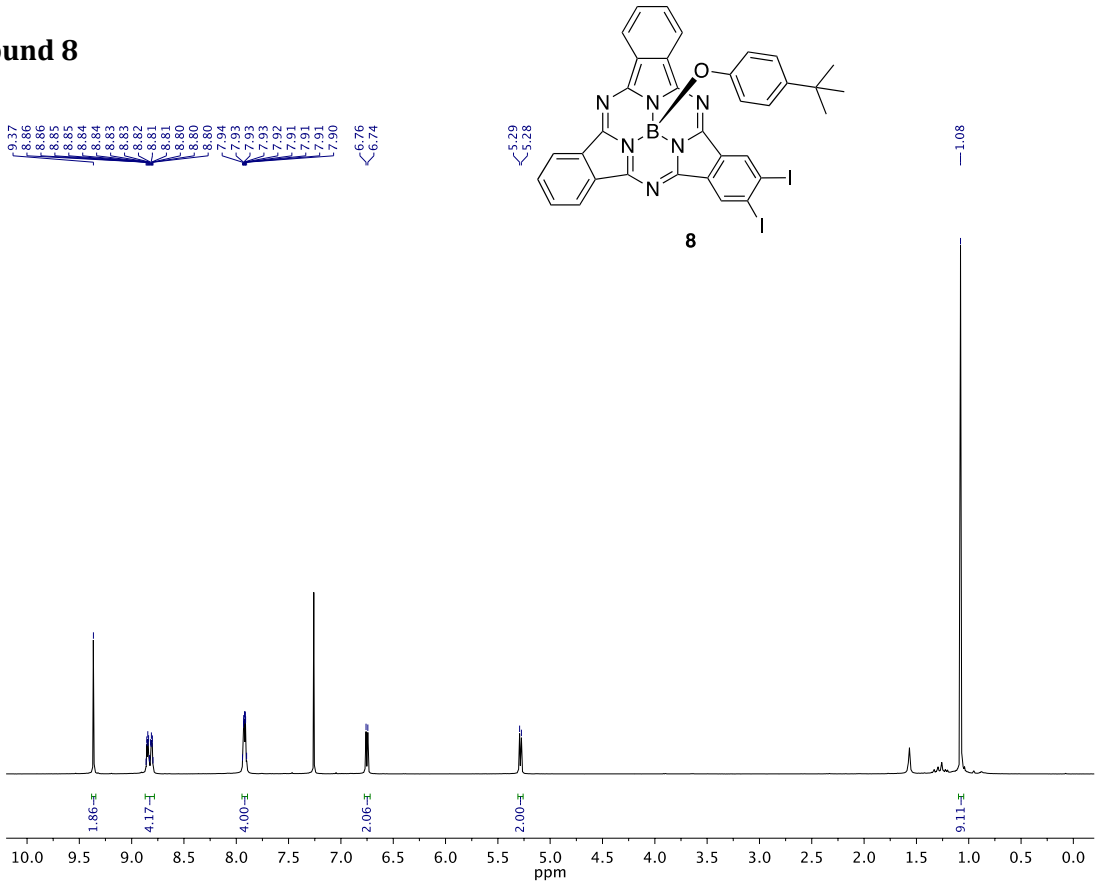


A suspension of K_2CO_3 (87.0 mg, 630 µmol) in CH_3OH (10 mL) was added to a solution of **10** (73.7 mg, 127 µmol) in THF (5 mL), and the mixture was stirred at rt for 40 min. Complete desilylation was indicated by TLC (70% CH_2Cl_2/heptane), and the mixture was filtered through a short plug (SiO_2, 40-63 µm, CH_2Cl_2). Toluene (10 mL) was added to the filtrate and the volume reduced to ca. 2-3 mL. Then more toluene (10 mL) was added, and the solution containing **11** was concentrated to ca. 5 mL and then flushed with argon for 5 min. Next, to a mixture of **8** (101 mg, 127 µmol), $Pd_2(dba)_3$ (57.5 mg, 62.8 µmol), CuI (12.1 mg, 63.5 µmol) and $AsPh_3$ (155 mg, 506 µmol) under Ar was added Ar-flushed toluene (5 mL) and Et_3N (5 mL). The solution of **11** was then added, and the mixture was stirred at rt for 28 h (within the first 15 min, the mixture changed color from pink to dark purple). The mixture was passed through a short plug (SiO_2, 40-63 µm, 50% EtOAc/toluene). The product was then purified by flash column chromatography (SiO_2, 40-63 µm, 5% EtOAc/toluene) two times, thereafter passed through a bio-beads column (bio-beads S-X3, CH_2Cl_2), before it was purified a second time by flash column chromatography (SiO_2, 40-63 µm, 5% EtOAc/toluene). To remove minor impurities, the product was dissolved in a small amount of CH_2Cl_2 and precipitated with CH_3OH. The fine precipitate was filtered on a Celite plug and redissolved by addition of CH_2Cl_2; the filtrate was collected and concentrated, providing **4** as a

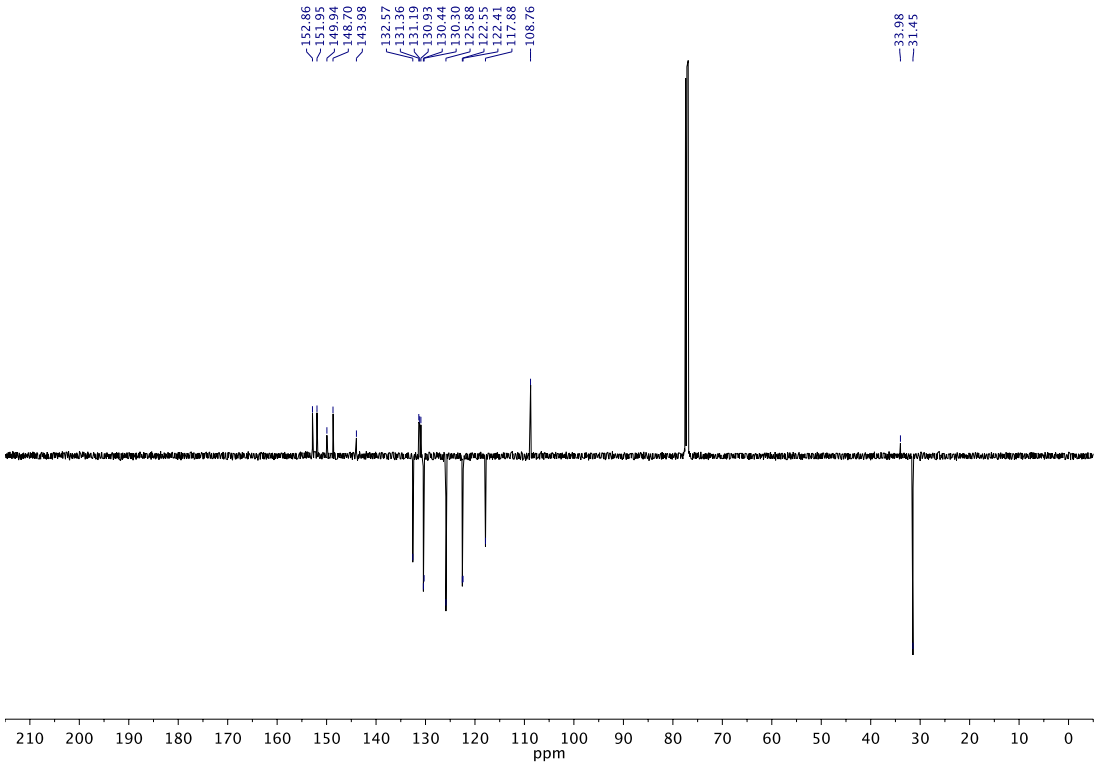
mixture of isomers (12.8 mg, 10%) as a green-red solid. Mp: >230 °C; TLC (5% EtOAc/PhMe): R_f = 0.50; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.01 (s, 4H), 8.86-8.82 (m, 4H), 8.79-8.75 (m, 4H), 7.95-7.89 (m, 8H), 6.80-6.74 (m, 4H), 5.36-5.31 (m, 4H), 1.41-1.32 (m, 84H), 1.10 (s, 9H), 1.08 (s, 9H) ppm; ^{13}C APT NMR (125 MHz, $CDCl_3$): δ 153.04, 152.14, 150.16, 150.10, 150.08, 150.06, 143.90, 131.55, 131.14, 130.34, 130.30, 130.20, 130.17, 129.62, 126.59, 126.58, 125.85, 125.82, 125.39, 125.36, 122.58, 122.24, 122.22, 119.04, 119.02, 117.94, 117.93, 116.76, 104.65, 104.63, 104.35, 104.29, 97.62, 97.60, 93.13, 93.10, 31.47, 31.45, 29.86, 19.11, 19.09, 19.06, 11.78, 11.75 ppm; HRMS (MALDI+): *m/z* = 1954.9958 [M+H$^+$], calcd for $^{12}C_{123}{}^{13}C_1H_{130}B_2N_{12}O_2Si_4^+$: *m/z* = 1954.9809. λ_{max}/nm ($\varepsilon/10^5$ $M^{-1}cm^{-1}$) (CH_2Cl_2): 314 (6.3), 445 (3.1), 507 (2.2), 552 (3.4), 576 (shoulder, 4.1), 621 (8.7).

NMR spectra

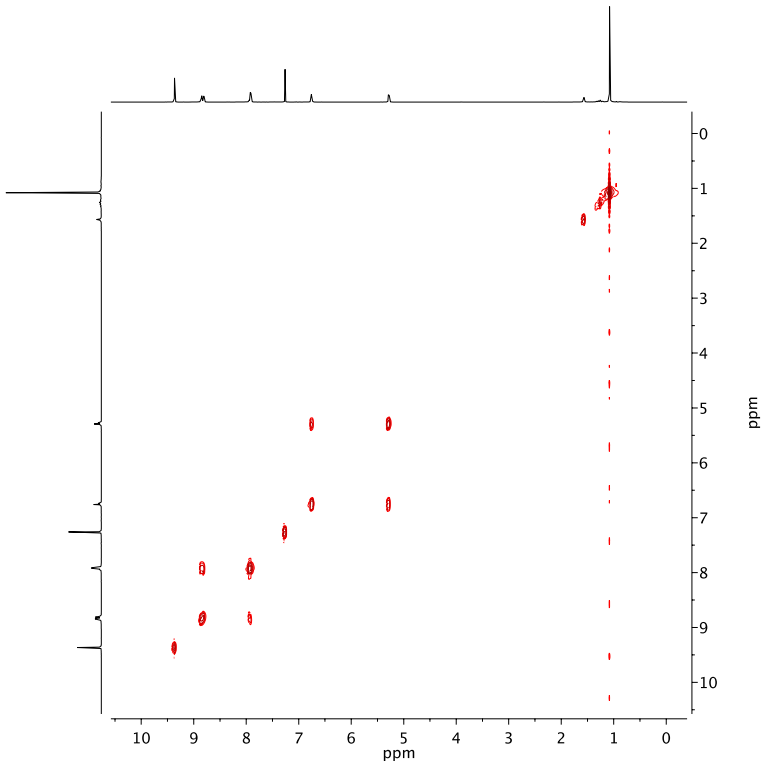
Compound 8



^{1}H NMR (500 MHz) spectrum of compound **8** recorded in $CDCl_3$.

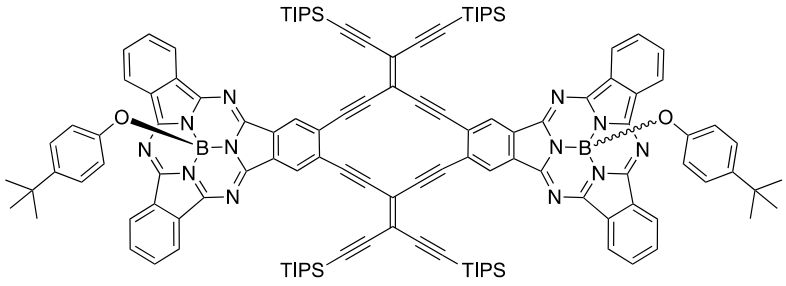


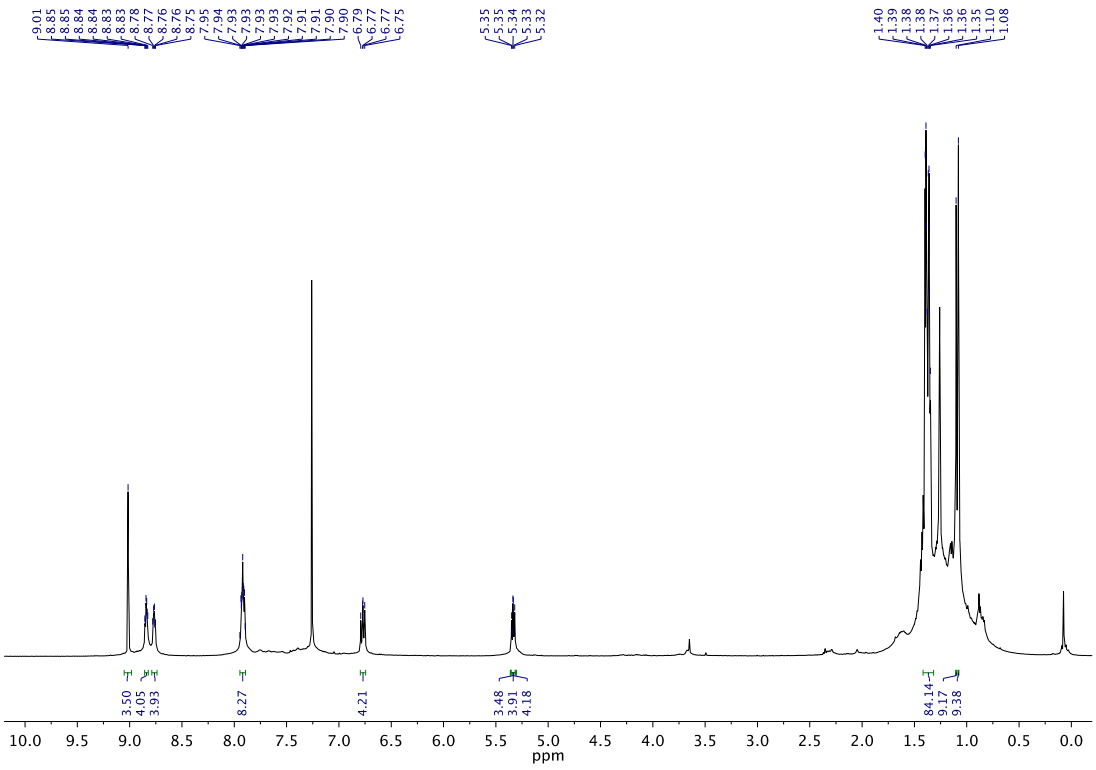
^{13}C APT NMR (125 MHz) spectrum of compound **8** recorded in $CDCl_3$.



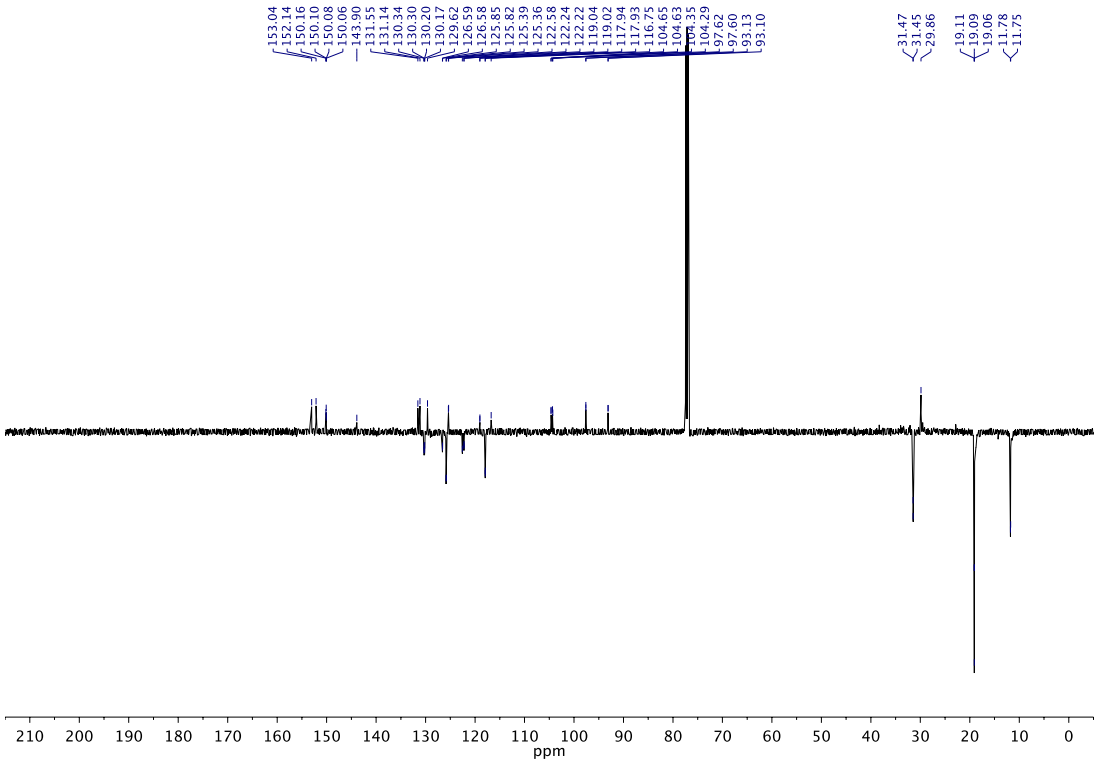
$^{1}H/^{1}H$ COSY (500 MHz) spectrum of compound **8** recorded in $CDCl_3$.

SubPc-Radiaannulene 4 (mixture of diastereoisomers)

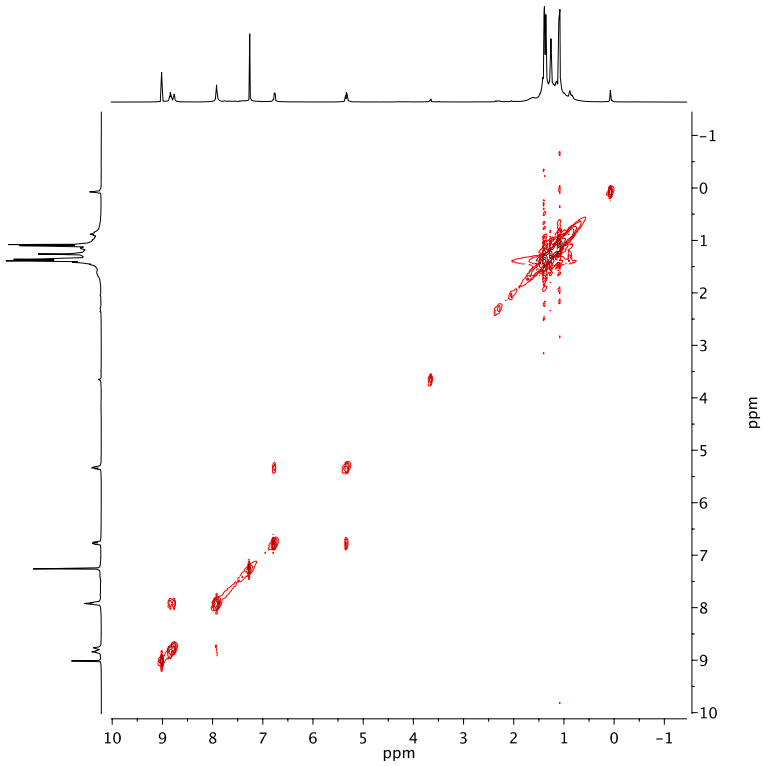




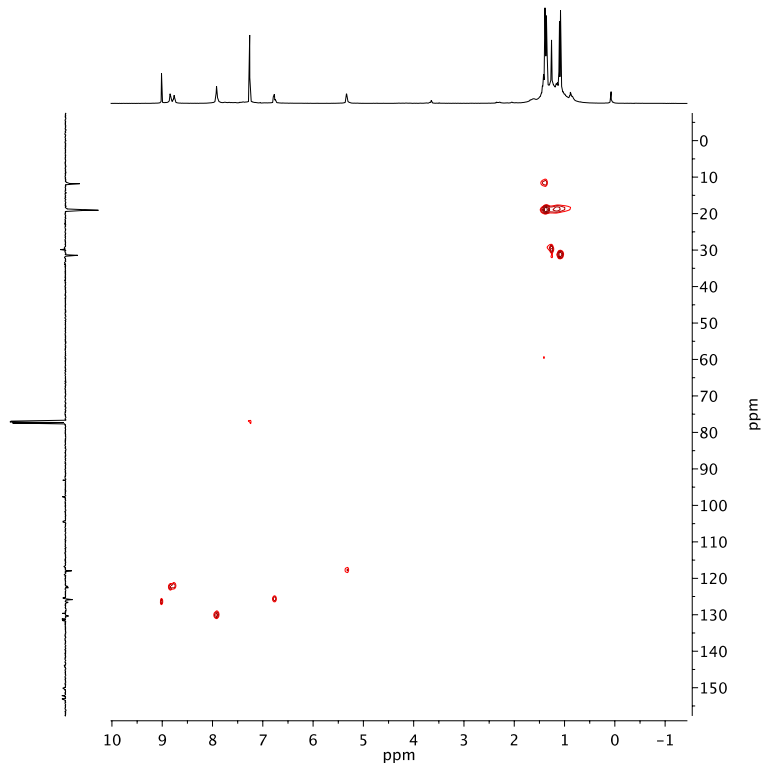
^{1}H NMR (500 MHz) spectrum of compound **4** recorded in $CDCl_3$.



^{13}C APT NMR (125 MHz) spectrum of compound **4** recorded in $CDCl_3$.



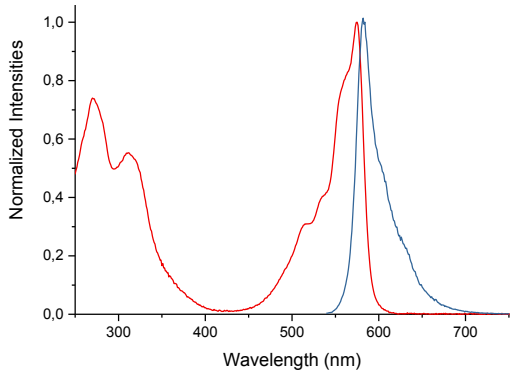
$^{1}H/^{1}H$ COSY (500 MHz) spectrum of compound **4** recorded in $CDCl_3$.



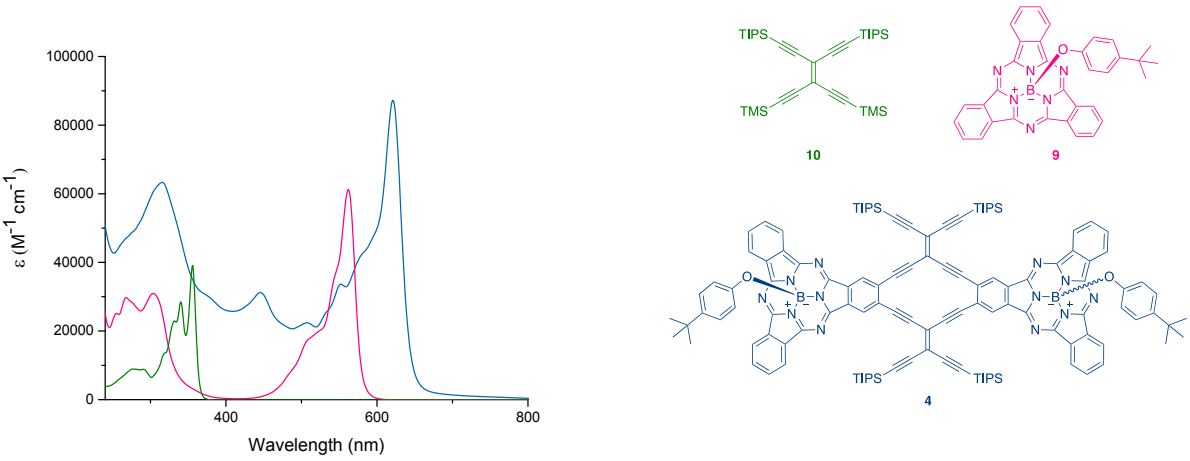
$^{1}H/^{13}C$ HSQC (500/125 MHz) spectrum of compound **4** recorded in $CDCl_3$.

UV-Vis absorption and emission spectra

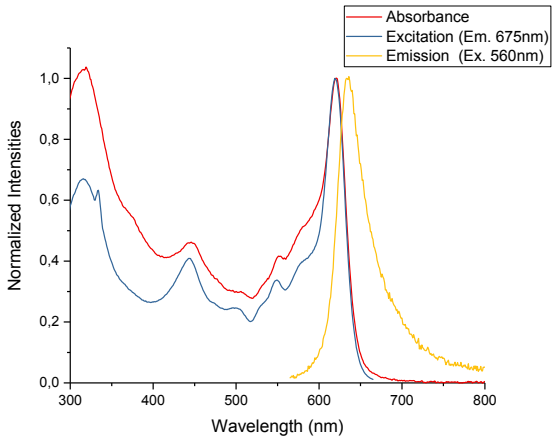
Solvents used for spectroscopic measurements were of highest purity grade and used as received. The UV-Vis absorption spectra were recorded on a Perkin-Elmer Lambda 1050 UV/vis/NIR double beam spectrometer using the pure solvent as baseline. The spectra were recorded in 1 cm path length cuvettes using slit widths of 1 nm and 1 nm steps. Molar absorptivities were determined according to Lambert-Beer's law. The values were determined as the average value of measurements performed on two different stock solutions. Emission spectra were measured using FluoroTime 300 (PicoQuant, Berlin, Germany) system with a 561 nm laser as excitation source. Excitation spectra were measured using a QuantaMaster400 from PTI.



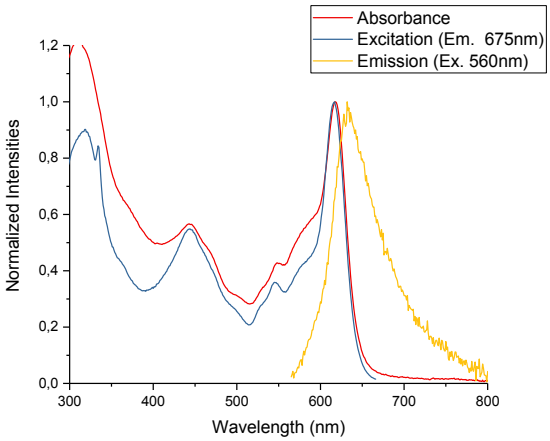
Normalized absorption (red) and emission (blue) spectra of compound **8** in CH_2Cl_2 with λ_{max} = 575 nm and Em_{max} = 582 nm.



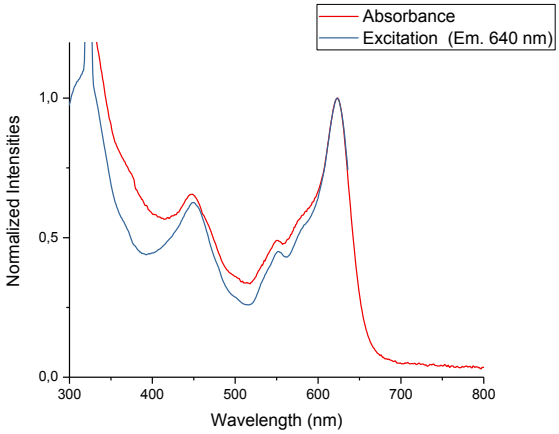
UV-Vis absorption spectra of compounds **4** (blue curve), **9** (pink curve) and **10** (green curve) dissolved in CH_2Cl_2.



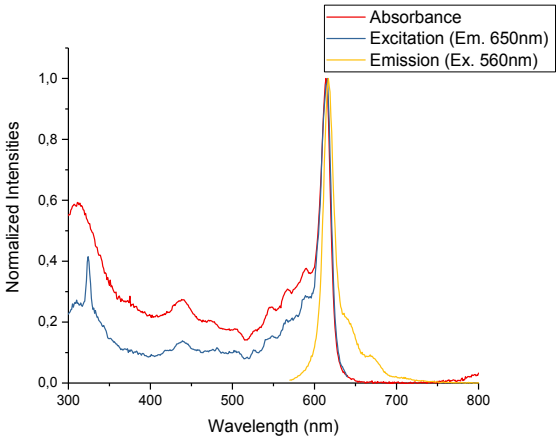
Normalized absorption (red), excitation (blue) and emission (yellow) spectra of compound **4** in CH_2Cl_2 with λ_{max} = 621 nm and Em_{max} = 635 nm.



Normalized absorption (red), excitation (blue) and emission (yellow) spectra of compound **4** in EtOH with λ_{max} = 617 nm and Em_{max} = 632 nm.



Normalized absorption (red) and excitation (blue) spectra of compound **4** in MeCN with λ_{max} = 623 nm. Emission spectrum not reported due to low resolution.



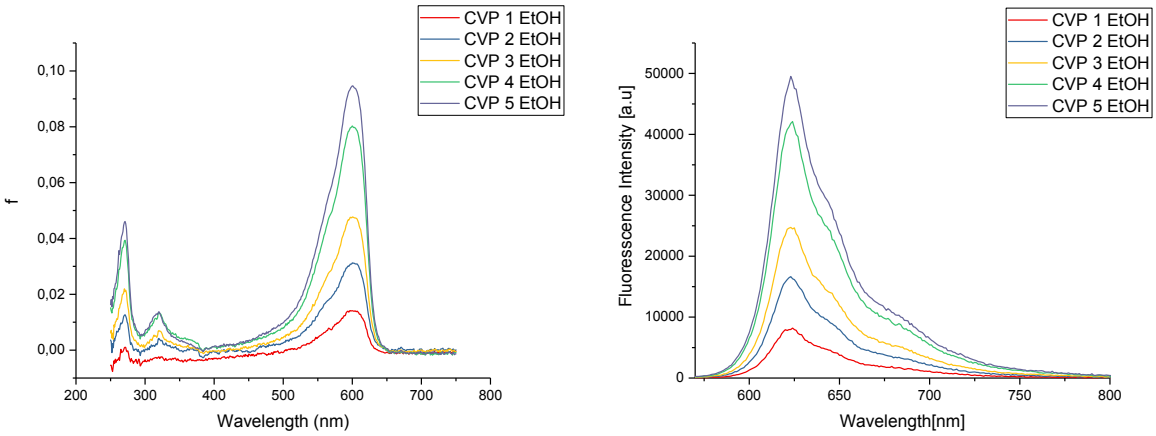
Normalized absorption (red) and emission (blue) spectra of compound **4** in heptane with λ_{max} = 614 nm and Em_{max} = 618 nm.

Fluorescence Quantum Yields

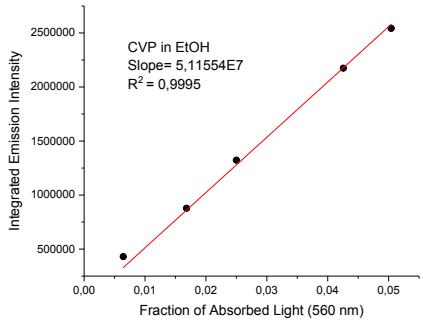
Fluorescence quantum yields were determined by the relative method.[1] Fluorescence quantum yields (QY) were measured on a Lambda 1050 (PerkinElmer) instrument for all absorption measurements and a Fluotime 300 (PicoQuant) instrument for all fluorescence measurements. Cresyl violet perchlorate (**CVP**) in ethanol was used as reference dye for quantum yield determination.[1] The emission measurements were performed in 1 cm cuvettes at 90° with respect to excitation light. Excitation wavelength 560 nm in all cases. Furthermore the absorption spectra were recorded after each fluorescence measurement in order to verify that no photobleaching of the sample had occurred during the fluorescence measurement. Due to low solubility of **4** in MeCN, measurements in this solvent were performed by first dissolving **4** in a small amount of CH_2Cl_2 and then diluting this solution with MeCN.

$$\Phi = \Phi_R \frac{Int}{Int_R} \cdot \frac{1 - 10^{-A_R}}{1 - 10^{-A}} \cdot \frac{n^2}{n_R^2}$$

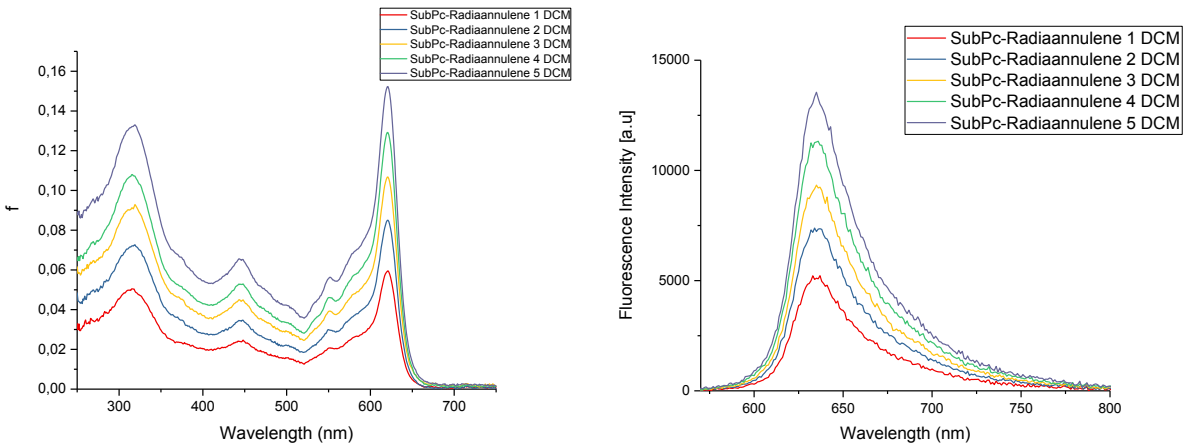
In the equation,[2] the quantum yield is given by Φ, while the quantum yield of the reference dye cresyl violet perchlorate is given by Φ_R and is measured to 0.54 in ethanol. *Int* is the integrated emission intensity and $1\text{-}10^{-A}$ is the fraction of absorbed light, where *A* is the absorbance measured at the wavelength of excitation and n is the refractive index of the solvent. Five data points were collected for all QY determinations with an absorbance measured below 0.1 for the longest wavelength absorption.



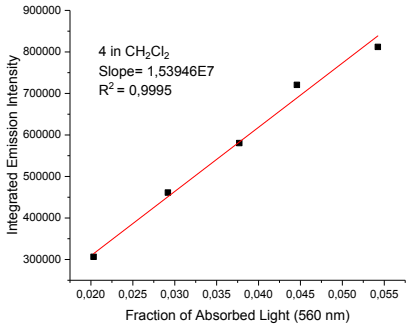
Fraction of absorbed light (left) and Emission spectra (right) for reference dye cresyl violet perchlorate (**CVP**) measured in EtOH at five different concentrations.



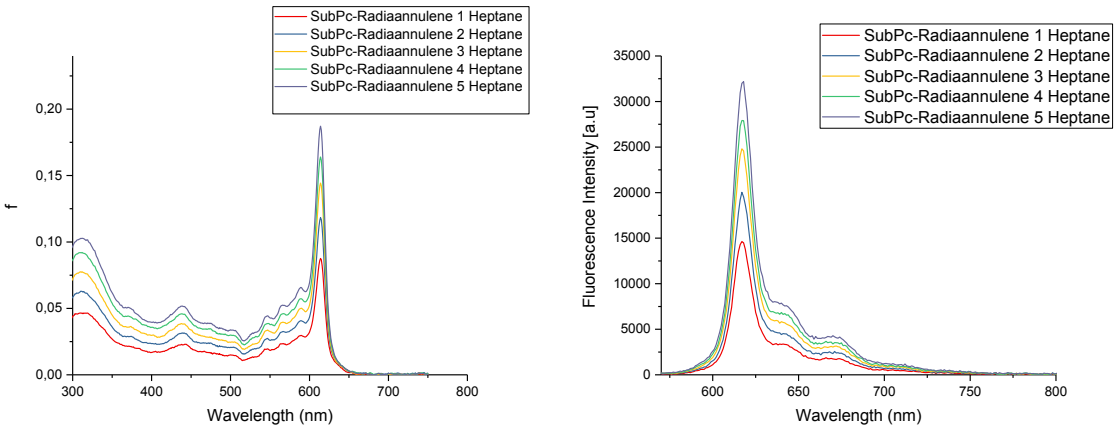
Linear-fit of the data points (I_{int} vs f_{a}) for **CVP** in EtOH.



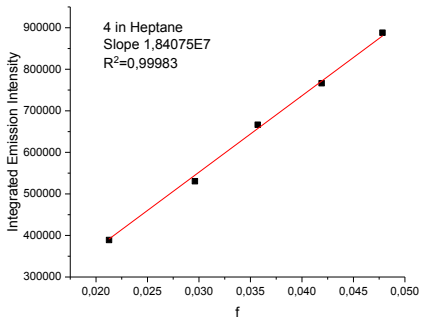
Fraction of absorbed light (left) and Emission spectra (right) for **4** measured in CH_2Cl_2 at five different concentrations.



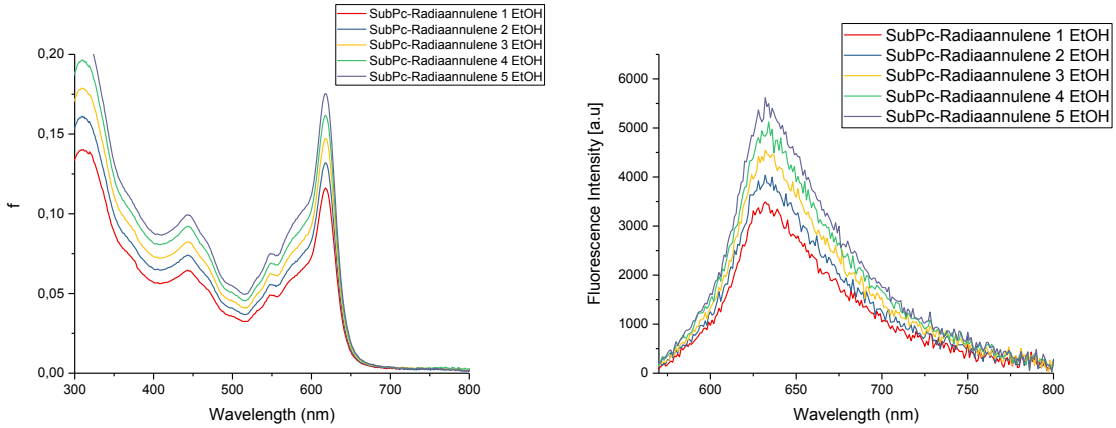
Linear-fit of the data points (I_{int} vs f_a) for **4** in CH_2Cl_2.



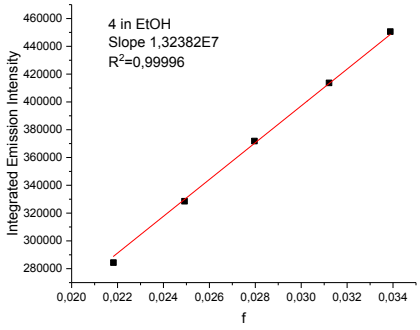
Fraction of absorbed light (left) and Emission spectra (right) for **4** measured in heptane at five different concentrations.



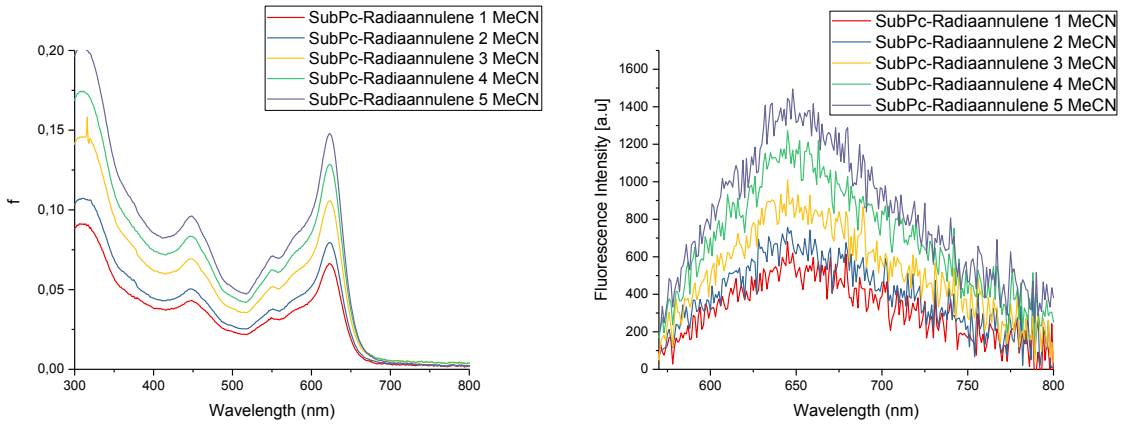
Linear-fit of the data points (I_{int} vs f_a) for **4** in heptane.



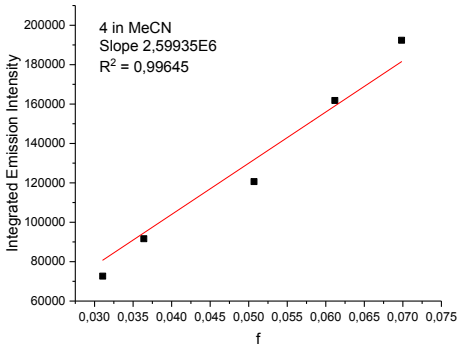
Fraction of absorbed light (left) and Emission spectra (right) for **4** measured in EtOH at five different concentrations.



Linear-fit of the data points (I_{int} vs f_a) for **4** in EtOH.



Fraction of absorbed light (left) and Emission spectra (right) for **4** measured in MeCN at five different concentrations.



Linear-fit of the data points (I_{int} vs f_a) for **4** in MeCN.

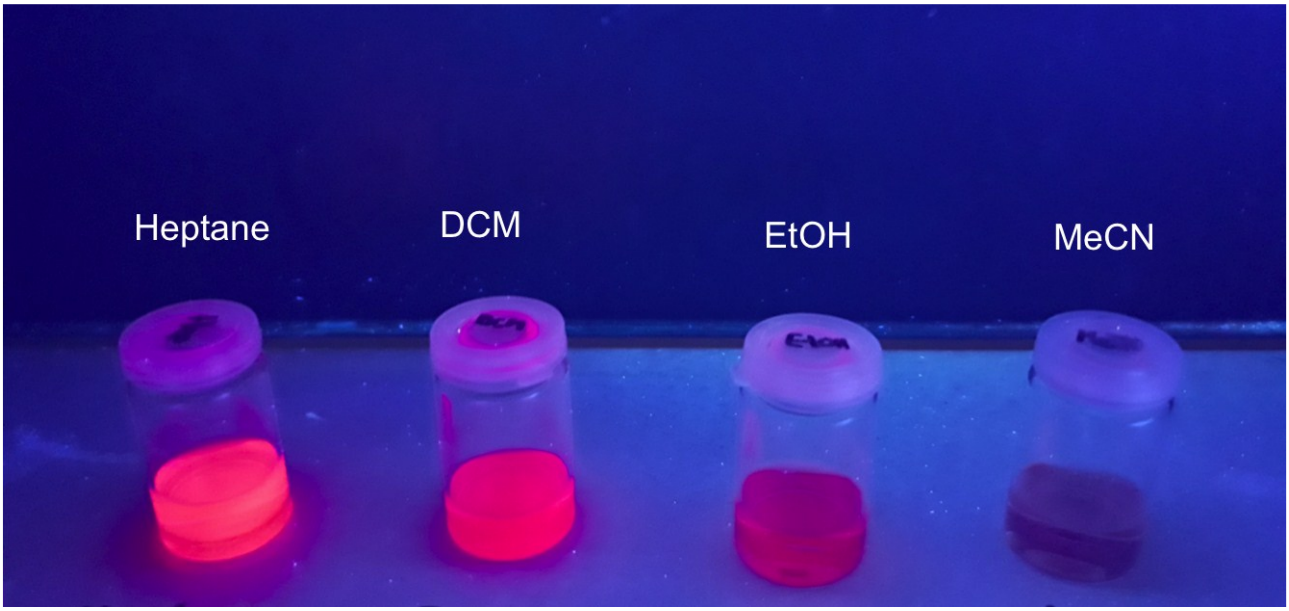


Photo of solutions of **4** in different solvents under irradiation with UV light (354 nm).

Cyclic voltammetry

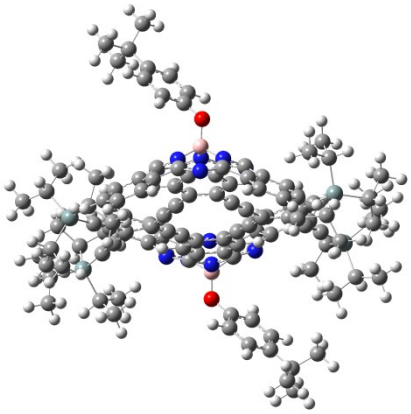
Cyclic voltammetry was carried out at room temperature in CH_2Cl_2 containing Bu_4NPF_6 (0.1 M) as the supporting electrolyte using an Autolab PGSTAT12 instrument driven by the Nova 1.11 software. The working electrode was a circular glassy carbon disk (d = 3 mm), the counter electrode was a thin platinum wire and the reference electrode was a silver wire immersed in the solvent-supporting electrolyte mixture and physically separated from the solution containing the substrate by a ceramic frit. The potential of the reference electrode was determined *vs* the ferrocene/ferrocenium (Fc/Fc^+) redox system in separate experiments. The voltage sweep rate was 0.1 Vs^{-1}. *iR*-Compensation was used in all experiments. Solutions were purged with argon saturated with CH_2Cl_2 for at least ten min before the measurements were made after which a stream of argon was maintained over the solutions. The formal potentials, $E^{o'}$, for the reversible one-electron transfers were determined as the average of the peak potentials for reduction and oxidation.

Computations

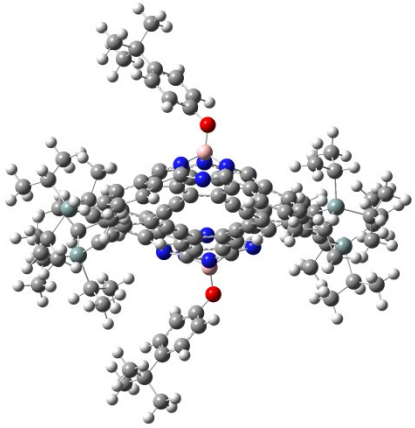
1. Isomers of 4 with TIPS groups

Computations were carried out at the DFT B3LYP/cc-pVDZ level of theory using computers hosted by the High Performance Computing Center at the University of Copenhagen. The Gaussian G09 suite of programs (Rev. E.01)[3] were used for the isomers of **4** with the TIPS included. The initial structures were generated by GaussView 5.0. True minima (opt=tight) resulted in all cases as evidenced by the absence of negative frequencies. Conformational analysis of the TIPS groups was deemed unnecessary and not carried out.

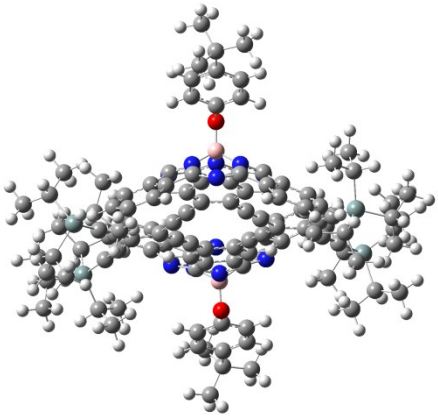
Structures of the isomers and conformations of 4 resulting from B3LYP/cc-pVDZ calculations. The abbreviations given in Italics refer to the two isomers, **4-*anti*** and **4-*syn***, and (in parentheses in Italics) the four conformations of the -O-Ph-*t*Bu groups for each of these.



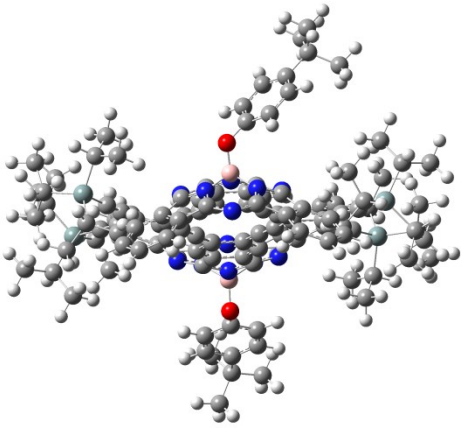
4-*anti* (*endo-endo-anti*)



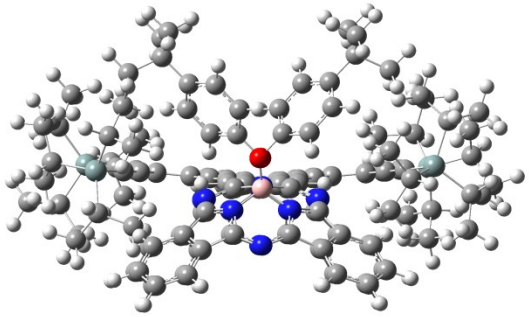
4-*anti* (*endo-endo-syn*)



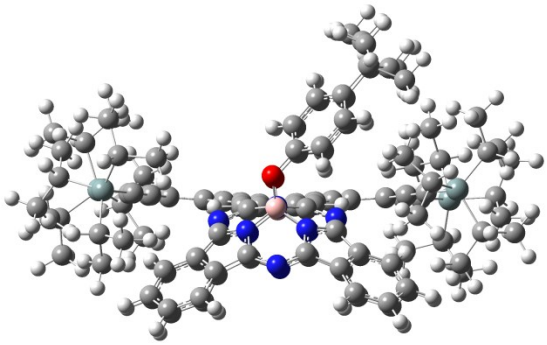
4-*anti* (*exo-exo*)



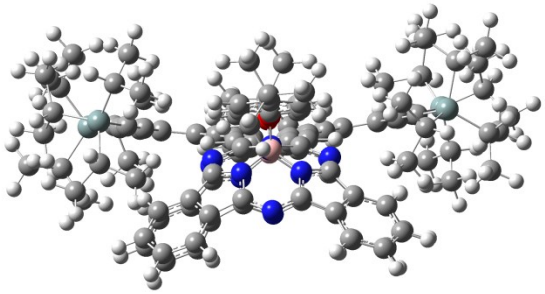
4-*anti* (*endo-exo*)



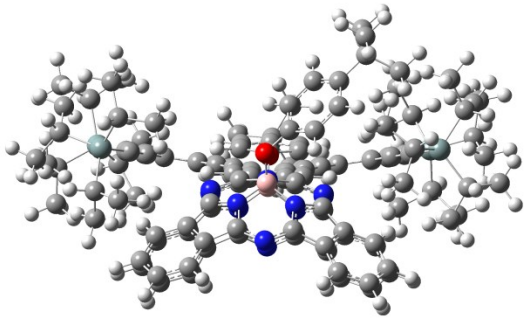
4-*syn* (*endo-endo-anti*)



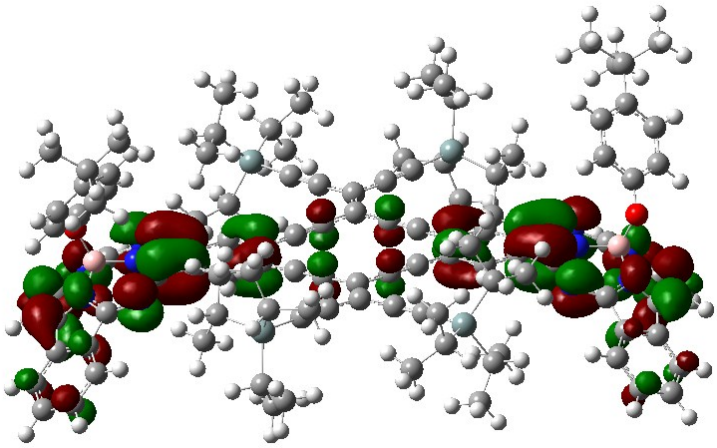
4-*syn* (*endo-endo-syn*)



4-*syn* (*exo-exo*)



4-*syn* (*endo-exo*)



LUMO of the **4-*syn*** dianion resulting from B3LYP/cc-pVDZ calculations.

G09 output (B3LYP/cc-pVDZ)

***4-anti* (*endo-endo-anti*)**


```
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***4-anti* (*endo-endo-syn*)**


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***4-anti* (*exo-exo*)**

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***4-anti* (*endo-exo*)**

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4-*syn* (*endo-endo-anti*)

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4-*syn* (*endo-endo-syn*)

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4-*syn* (*exo-exo*)

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4-*syn* (*endo-exo*)

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4-*syn* (*endo-endo-anti*) dianion

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2O2Si4)]\\@

2. Isomers of 4 with TIPS groups replaced by hydrogen atoms

Based on the investigation of conformers, the lowest energy *anti* (**4b**) and *syn* (**4a**) conformers were chosen for further investigation. The TIPS groups were replaced with H atoms in order to lower the computational time, as the system size proved demanding when calculating the linear response. The systems were further treated with *Gaussian16* (A.03)[4] using the functional BP86 and basis set 6-31G(d). To investigate the effect of solvent (CH_2Cl_2), the polarizable continuum model (PCM) as implemented in *Gaussian16* was used.

4a – vacuum BP86/6-31G(d)


```
1\1\GINC-NODE381\FOpt\RBP86\6-31G(d)\C88H50B2N12O2\ROOT\20-Dec-2017\0\
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4b -vacuum BP86/6-31G(d)


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2396255\H,3.8727982321,-5.7894536675,0.817029805\H,-2.3587795978,-6.53
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,54.7457514,9.8395576\PG=C01 [X(C88H50B2N12O2)]\\@

4a – CH_2Cl_2 BP86/6-31G(d)

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\C,-3.525079225,-0.3921370228,-0.1649686793\C,-4.8106792277,-0.9821325
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4b – CH_2Cl_2 Bp86/6-31G(d)

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 8307774\C,-11.3263153356,-5.4097472005,0.3587173846\C,-8.9695618618,-5
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```

Linear response calculations

From the re-optimized structures, the linear response was calculated either in vacuum or with PCM solvent effect depending on the method used for the geometry optimization. In order to gain insight into a large part of the visible spectrum, 200 states were calculated.

4a-vacuum BP86/6-31+G(d)

```
Excited State   1:      Singlet-A      1.3885 eV  892.95 nm  f=0.0079
<S**2>=0.000
     342 -> 346        0.12176
     342 -> 347        0.14884
     343 -> 346       -0.15482
     343 -> 347        0.11564
     344 -> 345        0.64801
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4240.55625483
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      1.4123 eV  877.91 nm  f=0.2066
<S**2>=0.000
     342 -> 345        0.65972
     344 -> 346        0.16162
     344 -> 347        0.18748

 Excited State   3:      Singlet-A      1.5587 eV  795.46 nm  f=0.0085
<S**2>=0.000
     340 -> 345        0.68234
     343 -> 345       -0.15267

 Excited State   4:      Singlet-A      1.5600 eV  794.75 nm  f=0.0001
<S**2>=0.000
     341 -> 345        0.70555

 Excited State   5:      Singlet-A      1.5960 eV  776.84 nm  f=0.1136
<S**2>=0.000
     340 -> 345        0.17479
```

```
     342 -> 348       -0.17222
     343 -> 345        0.48634
     343 -> 349       -0.10970
     344 -> 346       -0.32662
     344 -> 347        0.25695
     344 -> 350        0.11473

 Excited State   6:      Singlet-A      1.6644 eV  744.94 nm  f=0.0000
<S**2>=0.000
     343 -> 346        0.47001
     343 -> 347        0.51049

 Excited State   7:      Singlet-A      1.6892 eV  733.99 nm  f=0.0000
<S**2>=0.000
     342 -> 346        0.39216
     342 -> 347       -0.29623
     344 -> 348        0.49661

 Excited State   8:      Singlet-A      1.7080 eV  725.89 nm  f=0.0001
<S**2>=0.000
     339 -> 345        0.17351
     342 -> 346        0.15100
     342 -> 347        0.19397
     343 -> 346        0.43616
     343 -> 347       -0.42617
     343 -> 350        0.13746
     344 -> 349       -0.10194

 Excited State   9:      Singlet-A      1.7134 eV  723.60 nm  f=0.0663
<S**2>=0.000
     342 -> 348        0.30597
     343 -> 345        0.38052
     343 -> 349       -0.21563
     344 -> 346        0.33873
     344 -> 347       -0.27700
     344 -> 350        0.13700

 Excited State  10:      Singlet-A      1.7250 eV  718.77 nm  f=0.0414
<S**2>=0.000
     342 -> 349        0.10420
     343 -> 348        0.61626
     344 -> 346       -0.20371
     344 -> 347       -0.24536

 Excited State  11:      Singlet-A      1.8056 eV  686.68 nm  f=0.9843
<S**2>=0.000
     342 -> 345       -0.21229
     342 -> 349       -0.21859
     343 -> 348        0.33921
     344 -> 346        0.33304
     344 -> 347        0.41699

 Excited State  12:      Singlet-A      1.8826 eV  658.57 nm  f=0.0165
<S**2>=0.000
     340 -> 346       -0.11132
     342 -> 346       -0.29458
     342 -> 347       -0.36982
     343 -> 346        0.14575
     343 -> 347       -0.11281
```

```
     343 -> 350        0.18066
     344 -> 345        0.16133
     344 -> 349        0.40706

 Excited State  13:      Singlet-A      1.9076 eV  649.96 nm  f=0.0001
<S**2>=0.000
     341 -> 346        0.70507

 Excited State  14:      Singlet-A      1.9089 eV  649.52 nm  f=0.0009
<S**2>=0.000
     340 -> 346        0.69493

 Excited State  15:      Singlet-A      1.9140 eV  647.78 nm  f=0.0018
<S**2>=0.000
     341 -> 347        0.70197

 Excited State  16:      Singlet-A      1.9144 eV  647.63 nm  f=0.0001
<S**2>=0.000
     340 -> 347        0.69686

 Excited State  17:      Singlet-A      1.9460 eV  637.12 nm  f=0.0061
<S**2>=0.000
     342 -> 348        0.35811
     343 -> 349        0.35905
     344 -> 346       -0.13233
     344 -> 347        0.11137
     344 -> 350        0.45109

 Excited State  18:      Singlet-A      1.9528 eV  634.89 nm  f=0.0000
<S**2>=0.000
     339 -> 348       -0.10444
     340 -> 347       -0.10533
     342 -> 346       -0.29826
     342 -> 347        0.24615
     342 -> 350        0.40420
     344 -> 348        0.37898

 Excited State  19:      Singlet-A      1.9659 eV  630.68 nm  f=0.0002
<S**2>=0.000
     339 -> 345        0.55434
     343 -> 350       -0.39290
     344 -> 349        0.18471

 Excited State  20:      Singlet-A      1.9941 eV  621.76 nm  f=0.0000
<S**2>=0.000
     341 -> 348        0.70591

 Excited State  21:      Singlet-A      1.9952 eV  621.41 nm  f=0.0015
<S**2>=0.000
     340 -> 348        0.70625

 Excited State  22:      Singlet-A      2.1207 eV  584.64 nm  f=0.0000
<S**2>=0.000
     336 -> 345        0.12018
     338 -> 345        0.68345

 Excited State  23:      Singlet-A      2.1491 eV  576.90 nm  f=0.1403
<S**2>=0.000
     339 -> 346       -0.33506
```

```
     339 -> 347        0.24334
     342 -> 348       -0.35208
     344 -> 346        0.14165
     344 -> 347       -0.10710
     344 -> 350        0.39497

 Excited State  24:      Singlet-A      2.1767 eV  569.60 nm  f=0.0482
<S**2>=0.000
     336 -> 345       -0.28410
     342 -> 346        0.21933
     342 -> 347        0.23971
     343 -> 346       -0.10079
     343 -> 350        0.27982
     344 -> 345       -0.17066
     344 -> 349        0.38616

 Excited State  25:      Singlet-A      2.1802 eV  568.70 nm  f=0.0091
<S**2>=0.000
     337 -> 345        0.68175
     342 -> 349       -0.13405

 Excited State  26:      Singlet-A      2.1951 eV  564.82 nm  f=0.0176
<S**2>=0.000
     336 -> 345        0.59454
     342 -> 347        0.15675
     342 -> 350       -0.16182
     343 -> 350        0.16223
     344 -> 349        0.16342

 Excited State  27:      Singlet-A      2.2001 eV  563.55 nm  f=0.3405
<S**2>=0.000
     337 -> 345        0.15470
     339 -> 346       -0.21549
     339 -> 347       -0.31788
     342 -> 349        0.53886
     344 -> 346        0.10074
     344 -> 347        0.11669

 Excited State  28:      Singlet-A      2.2021 eV  563.03 nm  f=0.0000
<S**2>=0.000
     336 -> 345        0.22186
     339 -> 348        0.33907
     342 -> 346        0.15927
     342 -> 347       -0.12807
     342 -> 350        0.47652
     344 -> 348       -0.21603

 Excited State  29:      Singlet-A      2.2131 eV  560.24 nm  f=0.0315
<S**2>=0.000
     337 -> 345       -0.10054
     339 -> 346        0.17483
     339 -> 347       -0.12067
     339 -> 350       -0.17434
     340 -> 349       -0.10282
     342 -> 348       -0.22711
     343 -> 345        0.21450
     343 -> 349        0.49419
     344 -> 346        0.16031
     344 -> 347       -0.14133
```

```
     344 -> 350       -0.10439

 Excited State  30:      Singlet-A      2.2784 eV  544.18 nm  f=0.0003
<S**2>=0.000
     341 -> 349        0.69980

 Excited State  31:      Singlet-A      2.2796 eV  543.89 nm  f=0.0041
<S**2>=0.000
     341 -> 350        0.70482

 Excited State  32:      Singlet-A      2.2801 eV  543.78 nm  f=0.0003
<S**2>=0.000
     340 -> 350        0.70051

 Excited State  33:      Singlet-A      2.2808 eV  543.59 nm  f=0.0006
<S**2>=0.000
     340 -> 349        0.69674

 Excited State  34:      Singlet-A      2.4254 eV  511.18 nm  f=0.3049
<S**2>=0.000
     338 -> 346       -0.14927
     338 -> 347        0.16096
     339 -> 346        0.34524
     339 -> 347        0.39942
     342 -> 349        0.30612
     344 -> 347        0.11032

 Excited State  35:      Singlet-A      2.4758 eV  500.78 nm  f=0.2326
<S**2>=0.000
     336 -> 346        0.14017
     338 -> 346        0.51246
     338 -> 347       -0.37784
     339 -> 346        0.14643

 Excited State  36:      Singlet-A      2.4870 eV  498.53 nm  f=0.1752
<S**2>=0.000
     336 -> 347        0.15224
     338 -> 346        0.33672
     338 -> 347        0.31146
     339 -> 346       -0.28103
     339 -> 347        0.24189
     339 -> 350       -0.15863
     342 -> 348        0.14221
     343 -> 349        0.10579
     344 -> 350       -0.18304

 Excited State  37:      Singlet-A      2.4906 eV  497.81 nm  f=0.0002
<S**2>=0.000
     337 -> 346       -0.15743
     339 -> 348        0.57096
     342 -> 346       -0.13147
     342 -> 347        0.10680
     342 -> 350       -0.20393
     344 -> 348        0.17822

 Excited State  38:      Singlet-A      2.5232 eV  491.38 nm  f=0.1690
<S**2>=0.000
     336 -> 346        0.51642
     336 -> 347        0.13317
```

```
     338 -> 346        0.11301
     338 -> 347        0.31250
     339 -> 347       -0.18584
     344 -> 350        0.10830

 Excited State  39:      Singlet-A      2.5283 eV  490.38 nm  f=0.0002
<S**2>=0.000
     337 -> 346        0.66416
     338 -> 348        0.15423
     339 -> 348        0.10665

 Excited State  40:      Singlet-A      2.5361 eV  488.88 nm  f=0.0007
<S**2>=0.000
     337 -> 347        0.69011

 Excited State  41:      Singlet-A      2.5468 eV  486.82 nm  f=0.0013
<S**2>=0.000
     337 -> 346       -0.13292
     338 -> 348        0.64286
     343 -> 350        0.12370

 Excited State  42:      Singlet-A      2.5481 eV  486.58 nm  f=0.1003
<S**2>=0.000
     336 -> 346       -0.26305
     336 -> 347        0.61638
     339 -> 347       -0.10017

 Excited State  43:      Singlet-A      2.5748 eV  481.53 nm  f=0.3175
<S**2>=0.000
     335 -> 345        0.10662
     336 -> 346        0.35946
     336 -> 347        0.26721
     338 -> 346       -0.24571
     338 -> 347       -0.33000
     339 -> 346       -0.15459
     339 -> 347        0.11279
     342 -> 348        0.10162
     343 -> 345        0.12220
     344 -> 350       -0.12131

 Excited State  44:      Singlet-A      2.5975 eV  477.31 nm  f=0.0143
<S**2>=0.000
     334 -> 345       -0.11570
     336 -> 348        0.13740
     338 -> 348        0.16250
     339 -> 345       -0.27355
     339 -> 349        0.36058
     342 -> 346        0.10809
     342 -> 347        0.11539
     343 -> 350       -0.27817
     344 -> 349        0.25549

 Excited State  45:      Singlet-A      2.6023 eV  476.44 nm  f=0.0191
<S**2>=0.000
     333 -> 345       -0.27129
     335 -> 345        0.63053

 Excited State  46:      Singlet-A      2.6081 eV  475.39 nm  f=0.0082
<S**2>=0.000
```

```
     333 -> 345        0.65045
     335 -> 345        0.24829

 Excited State  47:      Singlet-A      2.6095 eV  475.12 nm  f=0.0003
<S**2>=0.000
     334 -> 345        0.68822

 Excited State  48:      Singlet-A      2.6172 eV  473.73 nm  f=0.0290
<S**2>=0.000
     337 -> 348        0.69422

 Excited State  49:      Singlet-A      2.6281 eV  471.76 nm  f=0.0028
<S**2>=0.000
     336 -> 348        0.67740

 Excited State  50:      Singlet-A      2.6984 eV  459.47 nm  f=0.0278
<S**2>=0.000
     329 -> 345        0.22060
     332 -> 345        0.64077
     339 -> 350        0.11273

 Excited State  51:      Singlet-A      2.7055 eV  458.27 nm  f=0.0000
<S**2>=0.000
     330 -> 345       -0.26731
     331 -> 345        0.65308

 Excited State  52:      Singlet-A      2.7169 eV  456.35 nm  f=0.0000
<S**2>=0.000
     330 -> 345        0.64544
     331 -> 345        0.25804

 Excited State  53:      Singlet-A      2.7361 eV  453.14 nm  f=0.0046
<S**2>=0.000
     329 -> 345        0.60859
     332 -> 345       -0.17068
     338 -> 350        0.22996
     343 -> 351       -0.17779

 Excited State  54:      Singlet-A      2.8055 eV  441.94 nm  f=0.0000
<S**2>=0.000
     338 -> 349        0.65414
     344 -> 351       -0.21969

 Excited State  55:      Singlet-A      2.8176 eV  440.04 nm  f=0.0017
<S**2>=0.000
     324 -> 345       -0.14982
     327 -> 345       -0.22509
     339 -> 345        0.18241
     339 -> 349        0.50662
     343 -> 350        0.21935
     343 -> 356       -0.15504

 Excited State  56:      Singlet-A      2.8208 eV  439.53 nm  f=0.0009
<S**2>=0.000
     328 -> 345        0.69858

 Excited State  57:      Singlet-A      2.8315 eV  437.88 nm  f=0.0000
<S**2>=0.000
     327 -> 345        0.66158
```

```
     339 -> 349        0.16593

 Excited State  58:      Singlet-A      2.8349 eV  437.35 nm  f=0.0116
<S**2>=0.000
     338 -> 350        0.42140
     343 -> 351        0.54863

 Excited State  59:      Singlet-A      2.8406 eV  436.48 nm  f=0.0000
<S**2>=0.000
     325 -> 345        0.21672
     338 -> 349        0.22923
     344 -> 351        0.60254

 Excited State  60:      Singlet-A      2.8505 eV  434.96 nm  f=0.1848
<S**2>=0.000
     326 -> 345        0.31861
     339 -> 346       -0.10344
     339 -> 350        0.51265
     342 -> 351       -0.11060
     343 -> 345        0.11997
     343 -> 349        0.12559

 Excited State  61:      Singlet-A      2.8742 eV  431.38 nm  f=0.0006
<S**2>=0.000
     326 -> 345        0.59469
     336 -> 350       -0.12045
     339 -> 350       -0.27602

 Excited State  62:      Singlet-A      2.8750 eV  431.25 nm  f=0.0002
<S**2>=0.000
     325 -> 345        0.64608
     344 -> 351       -0.19369

 Excited State  63:      Singlet-A      2.8983 eV  427.78 nm  f=0.0450
<S**2>=0.000
     336 -> 350       -0.31889
     337 -> 349        0.58599
     338 -> 350       -0.12308
     343 -> 351        0.13340
     344 -> 352       -0.11729

 Excited State  64:      Singlet-A      2.9018 eV  427.26 nm  f=0.0000
<S**2>=0.000
     337 -> 350        0.70077

 Excited State  65:      Singlet-A      2.9021 eV  427.22 nm  f=0.0270
<S**2>=0.000
     336 -> 350        0.47221
     337 -> 349        0.37982
     338 -> 350        0.16356
     339 -> 350       -0.12748
     343 -> 351       -0.14899
     344 -> 352        0.20070

 Excited State  66:      Singlet-A      2.9087 eV  426.25 nm  f=0.0001
<S**2>=0.000
     336 -> 349        0.69913
```

```
 Excited State  67:      Singlet-A      2.9315 eV  422.94 nm  f=0.0609
<S**2>=0.000
     336 -> 350       -0.11544
     338 -> 350        0.11238
     342 -> 351        0.60561
     344 -> 352        0.21117

 Excited State  68:      Singlet-A      2.9340 eV  422.58 nm  f=0.0382
<S**2>=0.000
     336 -> 350       -0.34298
     338 -> 350        0.22731
     342 -> 351       -0.25646
     344 -> 352        0.46564

 Excited State  69:      Singlet-A      2.9462 eV  420.83 nm  f=0.0000
<S**2>=0.000
     333 -> 346        0.63506
     335 -> 346       -0.29876

 Excited State  70:      Singlet-A      2.9536 eV  419.77 nm  f=0.0004
<S**2>=0.000
     333 -> 346        0.13023
     333 -> 347        0.57477
     335 -> 346        0.18704
     335 -> 347       -0.31892

 Excited State  71:      Singlet-A      2.9574 eV  419.23 nm  f=0.0005
<S**2>=0.000
     333 -> 346        0.25735
     333 -> 347       -0.34824
     334 -> 348       -0.17518
     335 -> 346        0.48540
     335 -> 347       -0.15508

 Excited State  72:      Singlet-A      2.9629 eV  418.46 nm  f=0.0019
<S**2>=0.000
     334 -> 346        0.58137
     334 -> 347       -0.30339
     335 -> 348       -0.23058

 Excited State  73:      Singlet-A      2.9702 eV  417.42 nm  f=0.0002
<S**2>=0.000
     335 -> 347        0.10254
     343 -> 352        0.68934

 Excited State  74:      Singlet-A      2.9801 eV  416.05 nm  f=0.0059
<S**2>=0.000
     332 -> 346        0.12576
     333 -> 347        0.20834
     335 -> 346        0.29323
     335 -> 347        0.55387

 Excited State  75:      Singlet-A      2.9884 eV  414.88 nm  f=0.0154
<S**2>=0.000
     334 -> 346        0.32345
     334 -> 347        0.59438

 Excited State  76:      Singlet-A      2.9964 eV  413.78 nm  f=0.0002
<S**2>=0.000
```

```
     324 -> 345        0.66258

 Excited State  77:      Singlet-A      3.0312 eV  409.03 nm  f=0.0018
<S**2>=0.000
     333 -> 348        0.67132
     335 -> 348       -0.20903

 Excited State  78:      Singlet-A      3.0330 eV  408.79 nm  f=0.2412
<S**2>=0.000
     323 -> 345        0.59300
     338 -> 350        0.15552
     343 -> 351       -0.13893
     344 -> 352       -0.23957

 Excited State  79:      Singlet-A      3.0443 eV  407.26 nm  f=0.0002
<S**2>=0.000
     329 -> 347        0.15213
     332 -> 346       -0.31628
     342 -> 352        0.57357
     344 -> 355       -0.16356

 Excited State  80:      Singlet-A      3.0478 eV  406.81 nm  f=0.0025
<S**2>=0.000
     330 -> 346       -0.34630
     331 -> 346        0.58996
     335 -> 348       -0.13571

 Excited State  81:      Singlet-A      3.0554 eV  405.79 nm  f=0.0074
<S**2>=0.000
     329 -> 346        0.26852
     330 -> 348        0.17204
     331 -> 348        0.11646
     332 -> 346        0.43362
     332 -> 347       -0.36951
     342 -> 352        0.17109

 Excited State  82:      Singlet-A      3.0562 eV  405.68 nm  f=0.0048
<S**2>=0.000
     330 -> 347       -0.36372
     331 -> 347        0.57881
     335 -> 348        0.10858

 Excited State  83:      Singlet-A      3.0669 eV  404.27 nm  f=0.0148
<S**2>=0.000
     329 -> 348        0.14301
     330 -> 346        0.43522
     330 -> 347       -0.23253
     331 -> 346        0.29164
     331 -> 347       -0.17843
     332 -> 348        0.25216
     335 -> 348        0.19807

 Excited State  84:      Singlet-A      3.0731 eV  403.45 nm  f=0.0052
<S**2>=0.000
     330 -> 346       -0.18398
     330 -> 347        0.21423
     333 -> 348        0.16749
     334 -> 346        0.13293
     334 -> 347       -0.13726
```

```
     335 -> 348        0.50961
     340 -> 351       -0.23971

 Excited State  85:      Singlet-A      3.0748 eV  403.22 nm  f=0.0020
<S**2>=0.000
     329 -> 347       -0.28283
     332 -> 346       -0.25407
     332 -> 347       -0.19564
     334 -> 348        0.45716
     335 -> 346        0.13284
     341 -> 351        0.23342

 Excited State  86:      Singlet-A      3.0806 eV  402.46 nm  f=0.0012
<S**2>=0.000
     329 -> 347        0.24701
     331 -> 348       -0.11165
     332 -> 346        0.20507
     332 -> 347        0.40556
     334 -> 348        0.30591
     335 -> 347       -0.12194
     341 -> 351        0.23158
     344 -> 353       -0.11042

 Excited State  87:      Singlet-A      3.0830 eV  402.16 nm  f=0.0662
<S**2>=0.000
     322 -> 345        0.22745
     323 -> 345       -0.14338
     335 -> 348        0.18821
     340 -> 351        0.58614

 Excited State  88:      Singlet-A      3.0844 eV  401.98 nm  f=0.0000
<S**2>=0.000
     321 -> 345        0.66654
     322 -> 345       -0.10699
     329 -> 346        0.15608

 Excited State  89:      Singlet-A      3.0846 eV  401.94 nm  f=0.0065
<S**2>=0.000
     329 -> 346       -0.10179
     334 -> 348       -0.27873
     341 -> 351        0.61518

 Excited State  90:      Singlet-A      3.0851 eV  401.88 nm  f=0.0009
<S**2>=0.000
     321 -> 345        0.10482
     322 -> 345        0.64022
     340 -> 351       -0.25091

 Excited State  91:      Singlet-A      3.0961 eV  400.45 nm  f=0.0795
<S**2>=0.000
     320 -> 345        0.11592
     323 -> 345       -0.10530
     330 -> 346        0.31364
     330 -> 347        0.41317
     331 -> 346        0.19129
     331 -> 347        0.27153
     332 -> 348       -0.16608
```

```
 Excited State  92:      Singlet-A      3.1080 eV  398.92 nm  f=0.0000
<S**2>=0.000
     321 -> 345       -0.14709
     329 -> 346        0.49302
     329 -> 347       -0.13414
     332 -> 347        0.21171
     334 -> 348       -0.10312
     344 -> 353        0.30237

 Excited State  93:      Singlet-A      3.1135 eV  398.22 nm  f=0.2379
<S**2>=0.000
     323 -> 345        0.17202
     327 -> 346       -0.13016
     338 -> 350       -0.13652
     342 -> 353       -0.22737
     343 -> 351        0.11233
     344 -> 352        0.13096
     344 -> 354        0.52755

 Excited State  94:      Singlet-A      3.1157 eV  397.93 nm  f=0.0009
<S**2>=0.000
     321 -> 345        0.10880
     329 -> 346       -0.17660
     329 -> 347        0.11419
     331 -> 348       -0.13118
     334 -> 348        0.13505
     342 -> 354       -0.25449
     344 -> 353        0.54050

 Excited State  95:      Singlet-A      3.1177 eV  397.68 nm  f=0.6304
<S**2>=0.000
     322 -> 345       -0.10700
     323 -> 345       -0.25875
     329 -> 345       -0.11403
     329 -> 348       -0.11664
     338 -> 350        0.21804
     340 -> 351       -0.13871
     342 -> 353       -0.14728
     343 -> 351       -0.17628
     344 -> 352       -0.20964
     344 -> 354        0.33218
     344 -> 357       -0.11733

 Excited State  96:      Singlet-A      3.1221 eV  397.12 nm  f=0.0012
<S**2>=0.000
     318 -> 345        0.10014
     329 -> 346        0.18792
     329 -> 347        0.44777
     330 -> 348       -0.12203
     332 -> 346       -0.12107
     332 -> 347       -0.20092
     342 -> 352       -0.14826
     344 -> 355        0.33923

 Excited State  97:      Singlet-A      3.1292 eV  396.22 nm  f=0.0007
<S**2>=0.000
     343 -> 353        0.70128
```

```
 Excited State  98:      Singlet-A      3.1295 eV  396.18 nm  f=0.0001
<S**2>=0.000
     343 -> 354        0.70083

 Excited State  99:      Singlet-A      3.1343 eV  395.57 nm  f=0.0002
<S**2>=0.000
     328 -> 346        0.12998
     330 -> 348       -0.40376
     331 -> 348        0.54680

 Excited State 100:      Singlet-A      3.1560 eV  392.85 nm  f=0.0320
<S**2>=0.000
     320 -> 345        0.10802
     325 -> 346       -0.10048
     325 -> 347       -0.14887
     327 -> 346        0.14018
     329 -> 348       -0.31913
     330 -> 347        0.12954
     332 -> 348        0.44972
     343 -> 355        0.27064

 Excited State 101:      Singlet-A      3.1704 eV  391.06 nm  f=0.0382
<S**2>=0.000
     320 -> 345        0.23634
     325 -> 346        0.11978
     325 -> 347        0.13022
     329 -> 348        0.18254
     332 -> 348       -0.16153
     343 -> 355        0.57402

 Excited State 102:      Singlet-A      3.1736 eV  390.67 nm  f=0.0148
<S**2>=0.000
     319 -> 345        0.67961
     327 -> 346        0.14759

 Excited State 103:      Singlet-A      3.1760 eV  390.38 nm  f=0.0045
<S**2>=0.000
     318 -> 345        0.21328
     327 -> 348       -0.10278
     328 -> 346        0.48861
     328 -> 347       -0.12917
     330 -> 348       -0.20706
     331 -> 348       -0.23942
     342 -> 354        0.15987
     344 -> 355       -0.15511

 Excited State 104:      Singlet-A      3.1780 eV  390.13 nm  f=0.0006
<S**2>=0.000
     317 -> 345       -0.14638
     318 -> 345        0.41865
     326 -> 346       -0.10139
     326 -> 347        0.10592
     328 -> 346       -0.26292
     328 -> 347       -0.13094
     329 -> 347        0.10689
     342 -> 352       -0.13513
     342 -> 354       -0.12983
     344 -> 355       -0.36305
```

```
 Excited State 105:      Singlet-A      3.1796 eV  389.94 nm  f=0.0054
<S**2>=0.000
     319 -> 345       -0.16089
     327 -> 346        0.47087
     327 -> 347       -0.15817
     328 -> 348       -0.11460
     329 -> 348        0.32986
     332 -> 348        0.13972
     342 -> 353       -0.16058
     343 -> 355       -0.13324

 Excited State 106:      Singlet-A      3.1883 eV  388.87 nm  f=0.0019
<S**2>=0.000
     317 -> 345        0.11170
     318 -> 345        0.21310
     326 -> 346       -0.12899
     327 -> 348        0.10408
     328 -> 346        0.11576
     328 -> 347        0.59125
     331 -> 348        0.11188
     342 -> 354        0.11907

 Excited State 107:      Singlet-A      3.1931 eV  388.28 nm  f=0.0044
<S**2>=0.000
     320 -> 345        0.19881
     327 -> 346        0.24448
     327 -> 347        0.54136
     329 -> 348       -0.11129
     332 -> 348       -0.19233
     342 -> 353       -0.12163

 Excited State 108:      Singlet-A      3.2045 eV  386.91 nm  f=0.0070
<S**2>=0.000
     320 -> 345        0.14814
     325 -> 346        0.19179
     327 -> 346       -0.25779
     327 -> 347        0.20851
     328 -> 348        0.33961
     329 -> 348        0.28627
     330 -> 346       -0.10035
     332 -> 348        0.22604
     342 -> 353       -0.10929

 Excited State 109:      Singlet-A      3.2051 eV  386.84 nm  f=0.0191
<S**2>=0.000
     318 -> 345        0.14592
     326 -> 347        0.17073
     327 -> 348       -0.29629
     328 -> 346        0.22528
     328 -> 347       -0.15227
     330 -> 348        0.37311
     331 -> 348        0.20823
     342 -> 354       -0.13383
     344 -> 355        0.14391

 Excited State 110:      Singlet-A      3.2086 eV  386.41 nm  f=0.0008
<S**2>=0.000
     316 -> 345        0.56748
     317 -> 345        0.34874
```

```
     326 -> 346        0.15435

 Excited State 111:      Singlet-A      3.2140 eV  385.76 nm  f=0.0001
<S**2>=0.000
     316 -> 345       -0.40316
     317 -> 345        0.40556
     318 -> 345        0.12245
     326 -> 346        0.31015
     326 -> 347        0.12326
     342 -> 354       -0.10590

 Excited State 112:      Singlet-A      3.2167 eV  385.43 nm  f=0.0143
<S**2>=0.000
     312 -> 345       -0.17885
     320 -> 345        0.41134
     325 -> 346        0.11716
     325 -> 347        0.19928
     327 -> 347       -0.15840
     329 -> 348       -0.16301
     341 -> 352       -0.29371
     342 -> 353        0.20209
     343 -> 355       -0.16964

 Excited State 113:      Singlet-A      3.2190 eV  385.17 nm  f=0.0034
<S**2>=0.000
     320 -> 345        0.19809
     325 -> 347        0.10215
     341 -> 352        0.63605

 Excited State 114:      Singlet-A      3.2194 eV  385.11 nm  f=0.0010
<S**2>=0.000
     340 -> 352        0.69181

 Excited State 115:      Singlet-A      3.2213 eV  384.89 nm  f=0.0030
<S**2>=0.000
     325 -> 346        0.47767
     325 -> 347       -0.38910
     326 -> 348       -0.25117
     329 -> 348       -0.10409
     342 -> 355       -0.15333

 Excited State 116:      Singlet-A      3.2221 eV  384.79 nm  f=0.0003
<S**2>=0.000
     315 -> 345       -0.25844
     317 -> 345       -0.19167
     318 -> 345        0.25619
     325 -> 348       -0.17265
     326 -> 346        0.33572
     326 -> 347       -0.31304
     343 -> 356       -0.14271
     344 -> 355        0.14404

 Excited State 117:      Singlet-A      3.2333 eV  383.47 nm  f=0.0006
<S**2>=0.000
     315 -> 345        0.31309
     318 -> 345       -0.16407
     325 -> 348       -0.26466
     326 -> 346        0.25648
     326 -> 347       -0.18859
```

```
     327 -> 348       -0.14418
     329 -> 347        0.11084
     330 -> 348        0.12953
     342 -> 352       -0.14566
     343 -> 356        0.11016
     344 -> 355       -0.23222

 Excited State 118:      Singlet-A      3.2448 eV  382.10 nm  f=0.0007
<S**2>=0.000
     315 -> 345       -0.19493
     317 -> 345       -0.25627
     318 -> 345       -0.10021
     326 -> 346        0.19948
     326 -> 347        0.37070
     328 -> 347        0.15959
     330 -> 349        0.10280
     342 -> 354       -0.27774
     344 -> 353       -0.10322

 Excited State 119:      Singlet-A      3.2458 eV  381.99 nm  f=0.0825
<S**2>=0.000
     320 -> 345       -0.25091
     325 -> 346        0.25628
     325 -> 347        0.33624
     327 -> 346        0.13257
     327 -> 347        0.17004
     330 -> 347        0.10523
     332 -> 349       -0.11626
     335 -> 349       -0.11729
     342 -> 353        0.28838
     344 -> 354        0.10041

 Excited State 120:      Singlet-A      3.2510 eV  381.38 nm  f=0.0001
<S**2>=0.000
     315 -> 345        0.53115
     317 -> 345       -0.13448
     318 -> 345        0.16149
     326 -> 347        0.11281
     327 -> 348        0.12711
     342 -> 352        0.10830
     343 -> 356       -0.21688
     344 -> 355        0.18332

 Excited State 121:      Singlet-A      3.2664 eV  379.58 nm  f=0.0848
<S**2>=0.000
     325 -> 347       -0.12817
     326 -> 348       -0.24786
     342 -> 353        0.10837
     342 -> 355        0.60441

 Excited State 122:      Singlet-A      3.2884 eV  377.03 nm  f=0.0031
<S**2>=0.000
     326 -> 346        0.19352
     326 -> 347        0.27008
     335 -> 350       -0.26623
     342 -> 354        0.43634
     344 -> 353        0.20554
```

```
 Excited State 123:      Singlet-A      3.2886 eV  377.01 nm  f=0.0748
<S**2>=0.000
     325 -> 346       -0.18510
     325 -> 347       -0.24913
     329 -> 348        0.10726
     334 -> 350        0.23620
     342 -> 353        0.41769
     342 -> 355       -0.14697
     344 -> 354        0.20683
     344 -> 356        0.16557

 Excited State 124:      Singlet-A      3.3112 eV  374.44 nm  f=0.0179
<S**2>=0.000
     324 -> 346        0.31501
     324 -> 347       -0.13158
     327 -> 347       -0.11864
     328 -> 348        0.37679
     330 -> 350       -0.12330
     334 -> 350        0.21142
     335 -> 349        0.12332
     344 -> 356       -0.29959

 Excited State 125:      Singlet-A      3.3176 eV  373.71 nm  f=0.0055
<S**2>=0.000
     324 -> 346        0.31300
     324 -> 347       -0.30207
     328 -> 348       -0.27987
     330 -> 350        0.10764
     333 -> 349        0.13288
     334 -> 350       -0.19151
     335 -> 349       -0.10306
     344 -> 356       -0.29273

 Excited State 126:      Singlet-A      3.3181 eV  373.66 nm  f=0.0008
<S**2>=0.000
     327 -> 348        0.35895
     328 -> 347       -0.11018
     329 -> 347        0.10632
     329 -> 350        0.10348
     330 -> 348        0.14079
     332 -> 350        0.18612
     335 -> 350        0.42547
     342 -> 354        0.13067

 Excited State 127:      Singlet-A      3.3194 eV  373.51 nm  f=0.0045
<S**2>=0.000
     324 -> 347        0.11716
     333 -> 349        0.64986
     335 -> 349       -0.20644

 Excited State 128:      Singlet-A      3.3258 eV  372.79 nm  f=0.0001
<S**2>=0.000
     333 -> 350        0.68229
     335 -> 350       -0.11609

 Excited State 129:      Singlet-A      3.3390 eV  371.32 nm  f=0.0056
<S**2>=0.000
     325 -> 347        0.10465
     326 -> 348       -0.30906
```

```
     328 -> 348        0.10532
     333 -> 349        0.15600
     334 -> 350       -0.27669
     335 -> 349        0.44961
     342 -> 355       -0.10030

 Excited State 130:      Singlet-A      3.3419 eV  371.00 nm  f=0.0000
<S**2>=0.000
     325 -> 348       -0.28665
     327 -> 348        0.25714
     328 -> 346        0.11543
     334 -> 349        0.48904
     335 -> 350       -0.22650

 Excited State 131:      Singlet-A      3.3466 eV  370.48 nm  f=0.0310
<S**2>=0.000
     311 -> 345        0.34427
     314 -> 345       -0.29170
     324 -> 346       -0.25384
     326 -> 348       -0.16777
     334 -> 350        0.31896
     344 -> 356       -0.19081

 Excited State 132:      Singlet-A      3.3512 eV  369.97 nm  f=0.0145
<S**2>=0.000
     311 -> 345       -0.26909
     314 -> 345        0.24215
     324 -> 346       -0.18889
     328 -> 348       -0.14075
     333 -> 349        0.14259
     334 -> 350        0.21197
     335 -> 349        0.33227
     344 -> 356       -0.15763
     344 -> 357       -0.23018

 Excited State 133:      Singlet-A      3.3551 eV  369.54 nm  f=0.0066
<S**2>=0.000
     325 -> 348       -0.19544
     327 -> 348       -0.28329
     328 -> 346       -0.11026
     332 -> 350       -0.12071
     333 -> 350        0.14750
     334 -> 349        0.28320
     335 -> 350        0.36854
     342 -> 354        0.11092

 Excited State 134:      Singlet-A      3.3608 eV  368.92 nm  f=0.0267
<S**2>=0.000
     324 -> 346        0.28516
     324 -> 347        0.51899
     328 -> 348       -0.12076
     329 -> 349       -0.10339
     330 -> 350        0.12267
     332 -> 349        0.14723
     334 -> 350        0.17366
     344 -> 356       -0.10126

 Excited State 135:      Singlet-A      3.3774 eV  367.10 nm  f=0.0399
<S**2>=0.000
```

```
     312 -> 345        0.16728
     314 -> 345       -0.10314
     318 -> 346       -0.10769
     324 -> 346        0.27815
     324 -> 347       -0.16043
     325 -> 346        0.11697
     328 -> 348       -0.13243
     329 -> 348       -0.11516
     331 -> 350       -0.10394
     334 -> 350        0.19699
     335 -> 349        0.12191
     342 -> 353       -0.10024
     344 -> 356        0.33942

 Excited State 136:      Singlet-A      3.3851 eV  366.26 nm  f=0.0106
<S**2>=0.000
     323 -> 347       -0.13108
     325 -> 348        0.42894
     326 -> 346        0.17427
     326 -> 350       -0.14041
     331 -> 349       -0.16053
     334 -> 349        0.30727
     341 -> 353        0.10768
     342 -> 357        0.11603

 Excited State 137:      Singlet-A      3.3897 eV  365.76 nm  f=0.0007
<S**2>=0.000
     313 -> 345       -0.13131
     323 -> 346        0.44414
     323 -> 347       -0.30478
     324 -> 348       -0.30314
     342 -> 356       -0.27557

 Excited State 138:      Singlet-A      3.3934 eV  365.36 nm  f=0.0466
<S**2>=0.000
     311 -> 345        0.10696
     314 -> 345       -0.23666
     324 -> 347        0.16275
     325 -> 346        0.12928
     325 -> 347       -0.11040
     325 -> 350       -0.13376
     326 -> 348        0.36786
     330 -> 350       -0.12305
     332 -> 349        0.21126
     334 -> 350       -0.18507
     335 -> 349        0.12944
     344 -> 356       -0.12022

 Excited State 139:      Singlet-A      3.3980 eV  364.87 nm  f=0.0002
<S**2>=0.000
     340 -> 353        0.32019
     340 -> 354       -0.27527
     341 -> 353        0.44860
     341 -> 354       -0.34515

 Excited State 140:      Singlet-A      3.3982 eV  364.86 nm  f=0.0002
<S**2>=0.000
     340 -> 353       -0.30670
     340 -> 354       -0.35425
```

```
     341 -> 353        0.32149
     341 -> 354        0.41921

 Excited State 141:      Singlet-A      3.4010 eV  364.56 nm  f=0.0007
<S**2>=0.000
     313 -> 345       -0.12603
     323 -> 346        0.20706
     323 -> 347       -0.16544
     324 -> 348        0.20458
     332 -> 350       -0.14653
     340 -> 354       -0.33091
     341 -> 353       -0.22174
     342 -> 356        0.39914

 Excited State 142:      Singlet-A      3.4037 eV  364.26 nm  f=0.0107
<S**2>=0.000
     312 -> 345        0.11402
     340 -> 353        0.52586
     341 -> 354        0.42625

 Excited State 143:      Singlet-A      3.4048 eV  364.14 nm  f=0.0108
<S**2>=0.000
     313 -> 345       -0.31926
     324 -> 348        0.13179
     334 -> 349       -0.11349
     340 -> 354        0.38132
     341 -> 353        0.32398
     342 -> 356        0.22914

 Excited State 144:      Singlet-A      3.4072 eV  363.89 nm  f=0.0045
<S**2>=0.000
     313 -> 345        0.51587
     314 -> 346        0.11592
     323 -> 346        0.17848
     323 -> 347       -0.15191
     329 -> 350        0.11758
     332 -> 350       -0.18332
     340 -> 354        0.16377
     341 -> 353        0.14563
     343 -> 357        0.10820

 Excited State 145:      Singlet-A      3.4152 eV  363.04 nm  f=0.0885
<S**2>=0.000
     312 -> 345        0.51741
     314 -> 345        0.15930
     320 -> 345        0.12985
     329 -> 349        0.13859
     332 -> 349        0.14991
     335 -> 349       -0.12232
     344 -> 356       -0.11114

 Excited State 146:      Singlet-A      3.4207 eV  362.45 nm  f=0.0145
<S**2>=0.000
     311 -> 345        0.45188
     312 -> 345       -0.14396
     313 -> 346        0.13896
     313 -> 347       -0.11855
     314 -> 345        0.42895
```

```
 Excited State 147:      Singlet-A      3.4227 eV  362.24 nm  f=0.0009
<S**2>=0.000
     323 -> 346        0.39435
     323 -> 347        0.52807
     331 -> 349       -0.15069

 Excited State 148:      Singlet-A      3.4242 eV  362.09 nm  f=0.0014
<S**2>=0.000
     323 -> 347        0.11632
     330 -> 349       -0.37058
     331 -> 349        0.53293

 Excited State 149:      Singlet-A      3.4287 eV  361.60 nm  f=0.0033
<S**2>=0.000
     330 -> 350       -0.32284
     331 -> 350        0.56021
     340 -> 355       -0.22313

 Excited State 150:      Singlet-A      3.4304 eV  361.43 nm  f=0.0026
<S**2>=0.000
     341 -> 355        0.68779

 Excited State 151:      Singlet-A      3.4317 eV  361.29 nm  f=0.0016
<S**2>=0.000
     330 -> 350       -0.12097
     331 -> 350        0.17504
     340 -> 355        0.65910

 Excited State 152:      Singlet-A      3.4327 eV  361.19 nm  f=0.0035
<S**2>=0.000
     313 -> 345        0.10342
     322 -> 347        0.13647
     323 -> 346        0.10233
     324 -> 348        0.11465
     332 -> 350        0.50791
     339 -> 351        0.24488
     341 -> 355        0.12656
     342 -> 356        0.10107
     343 -> 356        0.11600

 Excited State 153:      Singlet-A      3.4391 eV  360.52 nm  f=0.0003
<S**2>=0.000
     324 -> 348        0.50654
     330 -> 349        0.12083
     342 -> 356       -0.28682
     343 -> 357       -0.25218

 Excited State 154:      Singlet-A      3.4426 eV  360.14 nm  f=0.0155
<S**2>=0.000
     321 -> 346        0.62033
     322 -> 348       -0.16700
     329 -> 349       -0.10072
     344 -> 357       -0.15255

 Excited State 155:      Singlet-A      3.4435 eV  360.05 nm  f=0.0039
<S**2>=0.000
     321 -> 348       -0.19176
     322 -> 346        0.63316
     343 -> 356        0.10436
```

```
 Excited State 156:      Singlet-A      3.4497 eV  359.41 nm  f=0.0040
<S**2>=0.000
     310 -> 345       -0.20695
     321 -> 347        0.51664
     322 -> 348        0.10613
     329 -> 349       -0.17528
     330 -> 350       -0.18946
     332 -> 349       -0.22610
     344 -> 357       -0.10367

 Excited State 157:      Singlet-A      3.4507 eV  359.30 nm  f=0.0009
<S**2>=0.000
     322 -> 347        0.38744
     329 -> 350        0.33857
     330 -> 349        0.10254
     339 -> 351       -0.34176
     343 -> 356        0.17373

 Excited State 158:      Singlet-A      3.4528 eV  359.08 nm  f=0.0069
<S**2>=0.000
     307 -> 345        0.20195
     310 -> 345        0.17013
     320 -> 346        0.16653
     320 -> 347       -0.12143
     321 -> 347        0.11407
     322 -> 346       -0.12556
     322 -> 347       -0.30949
     342 -> 356        0.10184
     343 -> 356        0.36703

 Excited State 159:      Singlet-A      3.4528 eV  359.08 nm  f=0.0314
<S**2>=0.000
     310 -> 345        0.38865
     321 -> 346        0.13172
     321 -> 347        0.35657
     329 -> 349        0.16162
     330 -> 350        0.13170
     331 -> 350        0.11983
     343 -> 356       -0.15891
     344 -> 357        0.17938

 Excited State 160:      Singlet-A      3.4551 eV  358.85 nm  f=0.0141
<S**2>=0.000
     310 -> 345        0.49338
     312 -> 345        0.12599
     321 -> 346       -0.10635
     329 -> 349       -0.19940
     330 -> 350       -0.22540
     331 -> 350       -0.16944
     344 -> 357       -0.21524

 Excited State 161:      Singlet-A      3.4584 eV  358.50 nm  f=0.0027
<S**2>=0.000
     320 -> 347        0.13761
     321 -> 348       -0.10513
     322 -> 347       -0.34516
     329 -> 350        0.36469
     330 -> 349       -0.16547
```

```
     332 -> 350        0.21134
     339 -> 351       -0.24601
     343 -> 357        0.12951

 Excited State 162:      Singlet-A      3.4618 eV  358.15 nm  f=0.0137
<S**2>=0.000
     310 -> 345       -0.12159
     312 -> 345       -0.12689
     318 -> 347        0.15251
     321 -> 347        0.13522
     325 -> 350        0.10412
     326 -> 348       -0.10691
     330 -> 350       -0.12191
     331 -> 350       -0.13063
     332 -> 349        0.50740
     335 -> 349       -0.10351

 Excited State 163:      Singlet-A      3.4680 eV  357.51 nm  f=0.0001
<S**2>=0.000
     324 -> 348        0.14460
     342 -> 356       -0.19339
     343 -> 357        0.61461

 Excited State 164:      Singlet-A      3.4687 eV  357.44 nm  f=0.0001
<S**2>=0.000
     309 -> 345        0.67710
     330 -> 349       -0.13285

 Excited State 165:      Singlet-A      3.4693 eV  357.37 nm  f=0.0005
<S**2>=0.000
     309 -> 345        0.17948
     320 -> 346       -0.11508
     322 -> 347       -0.16941
     330 -> 349        0.45394
     331 -> 349        0.31443
     343 -> 356       -0.11477

 Excited State 166:      Singlet-A      3.4715 eV  357.15 nm  f=0.0001
<S**2>=0.000
     308 -> 345        0.69995

 Excited State 167:      Singlet-A      3.4739 eV  356.90 nm  f=0.0120
<S**2>=0.000
     317 -> 347        0.10965
     327 -> 350        0.18164
     329 -> 349        0.40733
     330 -> 350       -0.37299
     331 -> 350       -0.17435
     344 -> 357        0.13319

 Excited State 168:      Singlet-A      3.4881 eV  355.45 nm  f=0.0039
<S**2>=0.000
     323 -> 348        0.67862

 Excited State 169:      Singlet-A      3.5075 eV  353.48 nm  f=0.1145
<S**2>=0.000
     317 -> 346       -0.19613
     318 -> 346        0.10756
     318 -> 347        0.15872
```

```
     322 -> 348       -0.22752
     327 -> 350        0.14188
     329 -> 349       -0.29845
     339 -> 352       -0.24215
     344 -> 357        0.37109

 Excited State 170:      Singlet-A      3.5113 eV  353.10 nm  f=0.0000
<S**2>=0.000
     319 -> 346        0.69719

 Excited State 171:      Singlet-A      3.5186 eV  352.37 nm  f=0.0000
<S**2>=0.000
     319 -> 347        0.68211
     339 -> 351        0.10683

 Excited State 172:      Singlet-A      3.5325 eV  350.98 nm  f=0.0002
<S**2>=0.000
     319 -> 347       -0.16310
     320 -> 346       -0.14476
     327 -> 349        0.14198
     328 -> 350       -0.17380
     329 -> 350        0.35234
     332 -> 350       -0.14860
     339 -> 351        0.42324

 Excited State 173:      Singlet-A      3.5362 eV  350.61 nm  f=0.0005
<S**2>=0.000
     307 -> 345       -0.17811
     320 -> 346        0.18406
     320 -> 347       -0.11383
     321 -> 348        0.24988
     326 -> 350        0.19021
     338 -> 351        0.12593
     342 -> 357        0.51935

 Excited State 174:      Singlet-A      3.5466 eV  349.59 nm  f=0.0154
<S**2>=0.000
     315 -> 346       -0.14962
     316 -> 346        0.32553
     317 -> 346        0.12195
     317 -> 347       -0.12654
     318 -> 346        0.43959
     327 -> 350        0.28100
     328 -> 349       -0.18373

 Excited State 175:      Singlet-A      3.5483 eV  349.41 nm  f=0.0005
<S**2>=0.000
     307 -> 345       -0.14576
     317 -> 348       -0.17807
     320 -> 346        0.23086
     320 -> 347       -0.21039
     328 -> 350        0.47428
     329 -> 350        0.12469
     339 -> 351        0.13653
     342 -> 357       -0.17663

 Excited State 176:      Singlet-A      3.5493 eV  349.32 nm  f=0.0025
<S**2>=0.000
     315 -> 346        0.10856
```

```
     316 -> 346        0.56109
     317 -> 346        0.12214
     318 -> 346       -0.29603
     322 -> 348        0.15107

 Excited State 177:      Singlet-A      3.5528 eV  348.98 nm  f=0.0081
<S**2>=0.000
     315 -> 347        0.12128
     316 -> 346        0.11594
     316 -> 347        0.35460
     317 -> 346       -0.12216
     317 -> 347        0.26875
     318 -> 347       -0.28166
     327 -> 350       -0.22540
     328 -> 349       -0.29829

 Excited State 178:      Singlet-A      3.5554 eV  348.72 nm  f=0.0079
<S**2>=0.000
     315 -> 346        0.10835
     316 -> 347        0.34815
     317 -> 346        0.19947
     318 -> 347        0.38619
     322 -> 348       -0.26557
     326 -> 349       -0.14518
     328 -> 349       -0.14195
     339 -> 352        0.11080

 Excited State 179:      Singlet-A      3.5597 eV  348.30 nm  f=0.0053
<S**2>=0.000
     315 -> 346       -0.10240
     316 -> 347        0.35454
     318 -> 346        0.14588
     328 -> 349        0.52930

 Excited State 180:      Singlet-A      3.5612 eV  348.15 nm  f=0.0000
<S**2>=0.000
     317 -> 348        0.17174
     320 -> 346       -0.22741
     321 -> 348        0.34887
     327 -> 349        0.44402
     328 -> 350        0.17446

 Excited State 181:      Singlet-A      3.5624 eV  348.03 nm  f=0.0019
<S**2>=0.000
     316 -> 346       -0.18066
     316 -> 347        0.31095
     320 -> 348        0.13126
     322 -> 348        0.37802
     327 -> 350        0.38214

 Excited State 182:      Singlet-A      3.5633 eV  347.95 nm  f=0.0010
<S**2>=0.000
     315 -> 346       -0.10151
     315 -> 347       -0.10155
     316 -> 346        0.13143
     316 -> 347       -0.12071
     317 -> 346       -0.33663
     317 -> 347        0.20807
     318 -> 347        0.25804
```

```
     320 -> 348        0.38753
     339 -> 352        0.19388
     344 -> 357       -0.10011

 Excited State 183:      Singlet-A      3.5637 eV  347.91 nm  f=0.0007
<S**2>=0.000
     317 -> 348       -0.19885
     320 -> 347       -0.22513
     321 -> 348       -0.26543
     326 -> 350        0.13036
     327 -> 349        0.44138
     328 -> 350       -0.23551

 Excited State 184:      Singlet-A      3.5722 eV  347.08 nm  f=0.0023
<S**2>=0.000
     341 -> 356        0.69961

 Excited State 185:      Singlet-A      3.5729 eV  347.02 nm  f=0.0045
<S**2>=0.000
     340 -> 356        0.69209

 Excited State 186:      Singlet-A      3.5826 eV  346.07 nm  f=0.0009
<S**2>=0.000
     315 -> 346        0.33395
     315 -> 347        0.27479
     318 -> 347       -0.13331
     320 -> 348        0.17904
     322 -> 348       -0.21565
     325 -> 350        0.28248
     327 -> 350        0.28433

 Excited State 187:      Singlet-A      3.5869 eV  345.65 nm  f=0.0162
<S**2>=0.000
     307 -> 345        0.14079
     317 -> 348        0.23007
     320 -> 347        0.12205
     321 -> 348       -0.29717
     325 -> 349       -0.18458
     326 -> 350        0.31510
     328 -> 350        0.24947
     338 -> 351        0.16095
     342 -> 357        0.16638

 Excited State 188:      Singlet-A      3.5871 eV  345.64 nm  f=0.0128
<S**2>=0.000
     315 -> 346        0.38042
     315 -> 347       -0.35157
     317 -> 346       -0.14080
     317 -> 347       -0.17607
     326 -> 349        0.38867

 Excited State 189:      Singlet-A      3.5914 eV  345.22 nm  f=0.0003
<S**2>=0.000
     318 -> 348        0.27290
     320 -> 346       -0.17199
     320 -> 347       -0.20829
     325 -> 349        0.50327
     326 -> 350        0.14989
     327 -> 349       -0.12089
```

```
     328 -> 350        0.10381

 Excited State 190:      Singlet-A      3.5934 eV  345.03 nm  f=0.0011
<S**2>=0.000
     307 -> 345        0.46327
     312 -> 346       -0.10022
     317 -> 348       -0.15619
     326 -> 350       -0.25623
     338 -> 351        0.30696
     343 -> 356       -0.12153

 Excited State 191:      Singlet-A      3.5961 eV  344.77 nm  f=0.0011
<S**2>=0.000
     319 -> 348        0.69851

 Excited State 192:      Singlet-A      3.5991 eV  344.49 nm  f=0.0519
<S**2>=0.000
     315 -> 346       -0.26733
     315 -> 347       -0.30253
     325 -> 350        0.47191
     339 -> 352       -0.23131

 Excited State 193:      Singlet-A      3.6158 eV  342.89 nm  f=0.0372
<S**2>=0.000
     314 -> 348       -0.10781
     315 -> 346       -0.24673
     315 -> 347        0.29512
     317 -> 347       -0.14405
     318 -> 346       -0.22138
     318 -> 347        0.14044
     326 -> 349        0.41497

 Excited State 194:      Singlet-A      3.6253 eV  342.00 nm  f=0.0016
<S**2>=0.000
     314 -> 346        0.46385
     314 -> 347        0.48466

 Excited State 195:      Singlet-A      3.6282 eV  341.72 nm  f=0.0005
<S**2>=0.000
     313 -> 346        0.47663
     313 -> 347        0.51009

 Excited State 196:      Singlet-A      3.6334 eV  341.24 nm  f=0.0002
<S**2>=0.000
     311 -> 346       -0.10396
     314 -> 347       -0.16757
     315 -> 348       -0.20786
     316 -> 348       -0.26127
     317 -> 348       -0.14334
     318 -> 348        0.49514
     325 -> 349       -0.18422

 Excited State 197:      Singlet-A      3.6355 eV  341.04 nm  f=0.0000
<S**2>=0.000
     315 -> 348       -0.10015
     316 -> 348        0.63743
     318 -> 348        0.22311
```

```
 Excited State 198:      Singlet-A      3.6411 eV  340.51 nm  f=0.0094
<S**2>=0.000
     315 -> 346        0.15983
     315 -> 347        0.24491
     318 -> 346        0.18434
     318 -> 347        0.24002
     321 -> 350       -0.11837
     322 -> 348        0.22967
     325 -> 350        0.24710
     327 -> 350       -0.21574
     332 -> 349       -0.10390
     339 -> 352       -0.14732

 Excited State 199:      Singlet-A      3.6444 eV  340.20 nm  f=0.0088
<S**2>=0.000
     307 -> 345        0.20143
     312 -> 346       -0.22734
     312 -> 347        0.15026
     317 -> 348       -0.10683
     321 -> 348        0.16621
     325 -> 348        0.12904
     326 -> 350        0.41385
     342 -> 357       -0.17916

 Excited State 200:      Singlet-A      3.6613 eV  338.63 nm  f=0.0005
<S**2>=0.000
     304 -> 345        0.13008
     312 -> 346        0.17824
     314 -> 347        0.12161
     315 -> 348       -0.26712
     317 -> 349        0.18639
     320 -> 346        0.24714
     320 -> 347        0.31242
     325 -> 349        0.25439
     327 -> 349        0.11142
     330 -> 349        0.10981
```

4b – vacuum BP86/6-31+g(d)

```
Excited State   1:      Singlet-A      1.3884 eV  893.02 nm  f=0.0000
<S**2>=0.000
     342 -> 346       -0.12485
     342 -> 347       -0.14627
     343 -> 346       -0.15209
     343 -> 347        0.11903
     344 -> 345        0.64803
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4240.55629212
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      1.4123 eV  877.90 nm  f=0.2173
<S**2>=0.000
     342 -> 345        0.65966
     344 -> 346       -0.16475
     344 -> 347       -0.18533

 Excited State   3:      Singlet-A      1.5610 eV  794.28 nm  f=0.0118
<S**2>=0.000
```

```
     340 -> 345        0.60883
     341 -> 345       -0.29214
     343 -> 345        0.17699

 Excited State   4:      Singlet-A      1.5631 eV  793.20 nm  f=0.0004
<S**2>=0.000
     340 -> 345        0.29498
     341 -> 345        0.64136

 Excited State   5:      Singlet-A      1.5965 eV  776.59 nm  f=0.1147
<S**2>=0.000
     340 -> 345       -0.20028
     342 -> 348       -0.17146
     343 -> 345        0.47744
     343 -> 349       -0.10792
     344 -> 346       -0.31866
     344 -> 347        0.26185
     344 -> 350       -0.11313

 Excited State   6:      Singlet-A      1.6641 eV  745.06 nm  f=0.0000
<S**2>=0.000
     343 -> 346        0.47837
     343 -> 347        0.50307

 Excited State   7:      Singlet-A      1.6892 eV  733.99 nm  f=0.0000
<S**2>=0.000
     342 -> 346        0.38826
     342 -> 347       -0.30176
     344 -> 348        0.49628

 Excited State   8:      Singlet-A      1.7081 eV  725.84 nm  f=0.0000
<S**2>=0.000
     339 -> 345        0.17349
     342 -> 346        0.14961
     342 -> 347        0.19599
     343 -> 346       -0.42856
     343 -> 347        0.43301
     343 -> 350        0.13727
     344 -> 349        0.10222

 Excited State   9:      Singlet-A      1.7135 eV  723.58 nm  f=0.0679
<S**2>=0.000
     342 -> 348        0.30547
     343 -> 345        0.38015
     343 -> 349       -0.21571
     344 -> 346        0.33336
     344 -> 347       -0.28313
     344 -> 350       -0.13674

 Excited State  10:      Singlet-A      1.7251 eV  718.73 nm  f=0.0485
<S**2>=0.000
     342 -> 349        0.10454
     343 -> 348        0.61581
     344 -> 346        0.21010
     344 -> 347        0.24062

 Excited State  11:      Singlet-A      1.8057 eV  686.63 nm  f=1.0443
<S**2>=0.000
     342 -> 345        0.21255
```

```
     342 -> 349        0.21890
     343 -> 348       -0.33981
     344 -> 346        0.33905
     344 -> 347        0.41137

 Excited State  12:      Singlet-A      1.8825 eV  658.63 nm  f=0.0000
<S**2>=0.000
     342 -> 346        0.30320
     342 -> 347        0.36441
     343 -> 346        0.14386
     343 -> 347       -0.11712
     343 -> 350       -0.18137
     344 -> 345        0.16203
     344 -> 349        0.40862

 Excited State  13:      Singlet-A      1.9101 eV  649.09 nm  f=0.0010
<S**2>=0.000
     340 -> 346       -0.16274
     341 -> 346        0.68283

 Excited State  14:      Singlet-A      1.9115 eV  648.61 nm  f=0.0001
<S**2>=0.000
     340 -> 346        0.67667
     341 -> 346        0.16911

 Excited State  15:      Singlet-A      1.9168 eV  646.82 nm  f=0.0010
<S**2>=0.000
     340 -> 347        0.13878
     341 -> 347        0.68941

 Excited State  16:      Singlet-A      1.9180 eV  646.43 nm  f=0.0001
<S**2>=0.000
     340 -> 347        0.68379
     341 -> 347       -0.13836

 Excited State  17:      Singlet-A      1.9458 eV  637.18 nm  f=0.0068
<S**2>=0.000
     342 -> 348       -0.35836
     343 -> 349       -0.35840
     344 -> 346        0.13074
     344 -> 347       -0.11295
     344 -> 350        0.45015

 Excited State  18:      Singlet-A      1.9529 eV  634.86 nm  f=0.0000
<S**2>=0.000
     339 -> 348       -0.10412
     342 -> 346        0.29314
     342 -> 347       -0.25006
     342 -> 350        0.40304
     344 -> 348       -0.37778

 Excited State  19:      Singlet-A      1.9660 eV  630.63 nm  f=0.0000
<S**2>=0.000
     339 -> 345        0.55402
     343 -> 350       -0.39262
     344 -> 349       -0.18447

 Excited State  20:      Singlet-A      1.9971 eV  620.82 nm  f=0.0001
<S**2>=0.000
```

```
     341 -> 348        0.70574

 Excited State  21:      Singlet-A      1.9987 eV  620.33 nm  f=0.0016
<S**2>=0.000
     340 -> 348        0.70566

 Excited State  22:      Singlet-A      2.1220 eV  584.29 nm  f=0.0000
<S**2>=0.000
     336 -> 345       -0.11159
     338 -> 345        0.68449
     342 -> 350       -0.10004

 Excited State  23:      Singlet-A      2.1492 eV  576.89 nm  f=0.1472
<S**2>=0.000
     339 -> 346       -0.33082
     339 -> 347        0.24796
     342 -> 348        0.35293
     344 -> 346       -0.14053
     344 -> 347        0.10955
     344 -> 350        0.39443

 Excited State  24:      Singlet-A      2.1765 eV  569.66 nm  f=0.0000
<S**2>=0.000
     336 -> 345       -0.25239
     342 -> 346       -0.22645
     342 -> 347       -0.24223
     343 -> 346       -0.10044
     343 -> 350       -0.28777
     344 -> 345       -0.17451
     344 -> 349        0.39249

 Excited State  25:      Singlet-A      2.1830 eV  567.95 nm  f=0.0164
<S**2>=0.000
     337 -> 345        0.67006
     342 -> 349       -0.15825

 Excited State  26:      Singlet-A      2.1969 eV  564.35 nm  f=0.0001
<S**2>=0.000
     336 -> 345        0.60017
     339 -> 348       -0.11405
     342 -> 347       -0.14871
     342 -> 350       -0.17967
     343 -> 350       -0.14597
     344 -> 349        0.14518

 Excited State  27:      Singlet-A      2.2000 eV  563.57 nm  f=0.3663
<S**2>=0.000
     337 -> 345        0.17475
     339 -> 346       -0.20568
     339 -> 347       -0.31876
     342 -> 349        0.52614
     344 -> 346       -0.11006
     344 -> 347       -0.10535

 Excited State  28:      Singlet-A      2.2022 eV  563.01 nm  f=0.0029
<S**2>=0.000
     336 -> 345        0.24379
     339 -> 348        0.33317
     342 -> 346       -0.15707
```

```
     342 -> 347        0.12557
     342 -> 350        0.46610
     344 -> 348        0.21256

 Excited State  29:      Singlet-A      2.2127 eV  560.32 nm  f=0.0328
<S**2>=0.000
     337 -> 345        0.12170
     339 -> 346       -0.18543
     339 -> 347        0.10448
     339 -> 350       -0.17235
     340 -> 349        0.10277
     342 -> 348       -0.22543
     343 -> 345        0.21254
     343 -> 349        0.48941
     344 -> 346        0.15128
     344 -> 347       -0.14924
     344 -> 350        0.10294

 Excited State  30:      Singlet-A      2.2808 eV  543.60 nm  f=0.0004
<S**2>=0.000
     341 -> 349        0.69011

 Excited State  31:      Singlet-A      2.2826 eV  543.18 nm  f=0.0043
<S**2>=0.000
     341 -> 350        0.69328

 Excited State  32:      Singlet-A      2.2833 eV  543.00 nm  f=0.0005
<S**2>=0.000
     340 -> 349       -0.18773
     340 -> 350        0.67127

 Excited State  33:      Singlet-A      2.2840 eV  542.83 nm  f=0.0001
<S**2>=0.000
     340 -> 349        0.66376
     340 -> 350        0.16923
     341 -> 349       -0.10511

 Excited State  34:      Singlet-A      2.4258 eV  511.10 nm  f=0.3523
<S**2>=0.000
     338 -> 346       -0.14593
     338 -> 347        0.15697
     339 -> 346        0.35436
     339 -> 347        0.39327
     342 -> 349        0.30675
     344 -> 347       -0.10886

 Excited State  35:      Singlet-A      2.4771 eV  500.52 nm  f=0.2437
<S**2>=0.000
     336 -> 346       -0.12717
     338 -> 346        0.51250
     338 -> 347       -0.38660
     339 -> 346        0.13566

 Excited State  36:      Singlet-A      2.4875 eV  498.42 nm  f=0.1838
<S**2>=0.000
     336 -> 347       -0.14631
     338 -> 346        0.32524
     338 -> 347        0.31423
     339 -> 346       -0.28029
```

```
     339 -> 347        0.24997
     339 -> 350        0.16083
     342 -> 348       -0.14373
     343 -> 349       -0.10744
     344 -> 350       -0.18530

 Excited State  37:      Singlet-A      2.4914 eV  497.65 nm  f=0.0007
<S**2>=0.000
     337 -> 346        0.13852
     339 -> 348        0.57281
     342 -> 346        0.13047
     342 -> 347       -0.10930
     342 -> 350       -0.20490
     344 -> 348       -0.17919

 Excited State  38:      Singlet-A      2.5260 eV  490.83 nm  f=0.1783
<S**2>=0.000
     336 -> 346        0.52052
     336 -> 347        0.11962
     338 -> 346       -0.13003
     338 -> 347       -0.30533
     339 -> 347        0.18236
     344 -> 350       -0.10752

 Excited State  39:      Singlet-A      2.5309 eV  489.88 nm  f=0.0005
<S**2>=0.000
     337 -> 346        0.66591
     338 -> 348       -0.15305

 Excited State  40:      Singlet-A      2.5391 eV  488.29 nm  f=0.0002
<S**2>=0.000
     337 -> 347        0.68393
     338 -> 348        0.11511

 Excited State  41:      Singlet-A      2.5478 eV  486.64 nm  f=0.0010
<S**2>=0.000
     337 -> 346        0.13306
     337 -> 347       -0.12044
     338 -> 348        0.63390
     343 -> 350       -0.12558

 Excited State  42:      Singlet-A      2.5501 eV  486.20 nm  f=0.0987
<S**2>=0.000
     336 -> 346       -0.24709
     336 -> 347        0.62307

 Excited State  43:      Singlet-A      2.5744 eV  481.61 nm  f=0.3296
<S**2>=0.000
     335 -> 345       -0.10072
     336 -> 346        0.36707
     336 -> 347        0.25800
     338 -> 346        0.25346
     338 -> 347        0.32620
     339 -> 346        0.15354
     339 -> 347       -0.11547
     342 -> 348        0.10157
     343 -> 345        0.12216
     344 -> 350        0.12160
```

```
 Excited State  44:      Singlet-A      2.5978 eV  477.26 nm  f=0.0001
<S**2>=0.000
     334 -> 345        0.22560
     336 -> 348        0.10360
     337 -> 346       -0.10311
     338 -> 348       -0.16828
     339 -> 345       -0.26285
     339 -> 349        0.34536
     342 -> 346        0.10535
     342 -> 347        0.11205
     343 -> 350       -0.26593
     344 -> 349       -0.24618

 Excited State  45:      Singlet-A      2.6057 eV  475.81 nm  f=0.0029
<S**2>=0.000
     333 -> 345       -0.21540
     334 -> 345        0.60006
     335 -> 345       -0.20830
     339 -> 349       -0.12212

 Excited State  46:      Singlet-A      2.6059 eV  475.79 nm  f=0.0250
<S**2>=0.000
     334 -> 345        0.19606
     335 -> 345        0.64456

 Excited State  47:      Singlet-A      2.6139 eV  474.32 nm  f=0.0000
<S**2>=0.000
     333 -> 345        0.66277
     334 -> 345        0.21331

 Excited State  48:      Singlet-A      2.6204 eV  473.15 nm  f=0.0261
<S**2>=0.000
     337 -> 348        0.69644

 Excited State  49:      Singlet-A      2.6299 eV  471.44 nm  f=0.0002
<S**2>=0.000
     336 -> 348        0.68377

 Excited State  50:      Singlet-A      2.6960 eV  459.88 nm  f=0.0276
<S**2>=0.000
     329 -> 345        0.22206
     332 -> 345        0.64138
     339 -> 350        0.10578

 Excited State  51:      Singlet-A      2.7064 eV  458.12 nm  f=0.0026
<S**2>=0.000
     329 -> 345       -0.23675
     331 -> 345        0.66077

 Excited State  52:      Singlet-A      2.7142 eV  456.80 nm  f=0.0000
<S**2>=0.000
     330 -> 345        0.69321

 Excited State  53:      Singlet-A      2.7360 eV  453.15 nm  f=0.0049
<S**2>=0.000
     329 -> 345        0.57434
     331 -> 345        0.20829
     332 -> 345       -0.16414
     338 -> 350        0.22778
```

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     343 -> 351       -0.17785

 Excited State  54:      Singlet-A      2.8060 eV  441.85 nm  f=0.0000
<S**2>=0.000
     338 -> 349        0.64964
     344 -> 351        0.22529

 Excited State  55:      Singlet-A      2.8159 eV  440.30 nm  f=0.0000
<S**2>=0.000
     324 -> 345        0.11853
     328 -> 345        0.43587
     338 -> 349       -0.10279
     339 -> 345        0.14919
     339 -> 349        0.41775
     343 -> 350        0.17936
     343 -> 356        0.12600

 Excited State  56:      Singlet-A      2.8240 eV  439.04 nm  f=0.0000
<S**2>=0.000
     324 -> 345       -0.11295
     328 -> 345        0.54467
     339 -> 345       -0.12482
     339 -> 349       -0.33200
     343 -> 350       -0.14867
     343 -> 356       -0.10840

 Excited State  57:      Singlet-A      2.8317 eV  437.85 nm  f=0.0016
<S**2>=0.000
     327 -> 345        0.69813

 Excited State  58:      Singlet-A      2.8353 eV  437.28 nm  f=0.0128
<S**2>=0.000
     338 -> 350        0.41803
     343 -> 351        0.55409

 Excited State  59:      Singlet-A      2.8404 eV  436.50 nm  f=0.0000
<S**2>=0.000
     325 -> 345       -0.21159
     338 -> 349       -0.23716
     344 -> 351        0.60287

 Excited State  60:      Singlet-A      2.8506 eV  434.94 nm  f=0.1885
<S**2>=0.000
     326 -> 345        0.32227
     339 -> 346        0.10231
     339 -> 350        0.51315
     342 -> 351        0.11085
     343 -> 345        0.12006
     343 -> 349        0.12547

 Excited State  61:      Singlet-A      2.8747 eV  431.30 nm  f=0.0005
<S**2>=0.000
     326 -> 345        0.59145
     336 -> 350        0.10680
     339 -> 350       -0.28232

 Excited State  62:      Singlet-A      2.8754 eV  431.19 nm  f=0.0000
<S**2>=0.000
     325 -> 345        0.64521
```

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     344 -> 351        0.18953

 Excited State  63:      Singlet-A      2.9010 eV  427.39 nm  f=0.0485
<S**2>=0.000
     336 -> 350       -0.34090
     337 -> 349        0.56188
     338 -> 350        0.13761
     343 -> 351       -0.13748
     344 -> 352       -0.13618

 Excited State  64:      Singlet-A      2.9042 eV  426.91 nm  f=0.0214
<S**2>=0.000
     336 -> 350        0.43403
     337 -> 349        0.41235
     337 -> 350        0.15041
     338 -> 350       -0.15846
     339 -> 350        0.11044
     343 -> 351        0.13464
     344 -> 352        0.20127

 Excited State  65:      Singlet-A      2.9050 eV  426.80 nm  f=0.0020
<S**2>=0.000
     336 -> 350       -0.12458
     337 -> 350        0.68411

 Excited State  66:      Singlet-A      2.9105 eV  425.99 nm  f=0.0000
<S**2>=0.000
     336 -> 349        0.69946

 Excited State  67:      Singlet-A      2.9312 eV  422.98 nm  f=0.0628
<S**2>=0.000
     336 -> 350       -0.10736
     338 -> 350       -0.10512
     342 -> 351        0.61278
     344 -> 352        0.19636

 Excited State  68:      Singlet-A      2.9340 eV  422.58 nm  f=0.0376
<S**2>=0.000
     336 -> 350       -0.36123
     338 -> 350       -0.22851
     342 -> 351       -0.23757
     344 -> 352        0.46305

 Excited State  69:      Singlet-A      2.9464 eV  420.79 nm  f=0.0001
<S**2>=0.000
     333 -> 346       -0.37057
     334 -> 346        0.60007

 Excited State  70:      Singlet-A      2.9542 eV  419.69 nm  f=0.0003
<S**2>=0.000
     333 -> 347       -0.37434
     334 -> 347        0.59633

 Excited State  71:      Singlet-A      2.9578 eV  419.17 nm  f=0.0000
<S**2>=0.000
     333 -> 348       -0.14758
     334 -> 348       -0.12649
     335 -> 346        0.58406
     335 -> 347       -0.29555
```

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     343 -> 352        0.12933

 Excited State  72:      Singlet-A      2.9667 eV  417.92 nm  f=0.0023
<S**2>=0.000
     333 -> 346        0.49658
     333 -> 347       -0.29664
     334 -> 346        0.28252
     334 -> 347       -0.12623
     335 -> 348       -0.23878

 Excited State  73:      Singlet-A      2.9702 eV  417.43 nm  f=0.0000
<S**2>=0.000
     335 -> 347        0.11028
     343 -> 352        0.68683

 Excited State  74:      Singlet-A      2.9803 eV  416.01 nm  f=0.0000
<S**2>=0.000
     332 -> 346       -0.13522
     335 -> 346        0.31416
     335 -> 347        0.58485

 Excited State  75:      Singlet-A      2.9929 eV  414.26 nm  f=0.0235
<S**2>=0.000
     333 -> 346        0.28144
     333 -> 347        0.48640
     334 -> 346        0.19406
     334 -> 347        0.32914

 Excited State  76:      Singlet-A      3.0037 eV  412.78 nm  f=0.0000
<S**2>=0.000
     324 -> 345        0.66077
     332 -> 346       -0.10770

 Excited State  77:      Singlet-A      3.0237 eV  410.04 nm  f=0.1883
<S**2>=0.000
     323 -> 345        0.61368
     338 -> 350        0.13860
     343 -> 351       -0.12514
     344 -> 352        0.23294

 Excited State  78:      Singlet-A      3.0314 eV  409.01 nm  f=0.0000
<S**2>=0.000
     333 -> 348       -0.40742
     334 -> 348        0.57571

 Excited State  79:      Singlet-A      3.0432 eV  407.42 nm  f=0.0000
<S**2>=0.000
     329 -> 347        0.11154
     331 -> 346        0.22042
     332 -> 346       -0.36430
     342 -> 352        0.50789
     344 -> 355       -0.13849

 Excited State  80:      Singlet-A      3.0484 eV  406.72 nm  f=0.0000
<S**2>=0.000
     329 -> 346       -0.36335
     331 -> 346        0.47250
     332 -> 347        0.13126
     342 -> 352       -0.28567
```

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 Excited State  81:      Singlet-A      3.0528 eV  406.13 nm  f=0.0000
<S**2>=0.000
     329 -> 347        0.16451
     330 -> 348       -0.16219
     331 -> 346       -0.33399
     331 -> 347       -0.30526
     332 -> 346       -0.31381
     332 -> 347        0.34327

 Excited State  82:      Singlet-A      3.0583 eV  405.41 nm  f=0.0000
<S**2>=0.000
     329 -> 347       -0.29378
     330 -> 348       -0.13138
     331 -> 346       -0.15664
     331 -> 347        0.52113
     332 -> 346       -0.21095
     332 -> 347        0.14345
     342 -> 352       -0.10349

 Excited State  83:      Singlet-A      3.0652 eV  404.49 nm  f=0.0185
<S**2>=0.000
     329 -> 348        0.10992
     330 -> 346        0.53887
     330 -> 347       -0.32189
     332 -> 348        0.25743

 Excited State  84:      Singlet-A      3.0723 eV  403.56 nm  f=0.0095
<S**2>=0.000
     330 -> 347       -0.11763
     333 -> 346        0.11959
     333 -> 347       -0.12647
     335 -> 348        0.60615
     340 -> 351        0.17323

 Excited State  85:      Singlet-A      3.0754 eV  403.15 nm  f=0.0000
<S**2>=0.000
     329 -> 347        0.28985
     331 -> 347        0.23033
     332 -> 346        0.31298
     332 -> 347        0.35017
     333 -> 348        0.21895
     334 -> 348        0.15350
     335 -> 346        0.11191
     341 -> 351        0.12170
     342 -> 352        0.11408

 Excited State  86:      Singlet-A      3.0830 eV  402.16 nm  f=0.0000
<S**2>=0.000
     331 -> 346       -0.11304
     332 -> 347       -0.27091
     333 -> 348        0.34480
     334 -> 348        0.24138
     335 -> 347       -0.12352
     341 -> 351        0.36913
     344 -> 353       -0.12097

 Excited State  87:      Singlet-A      3.0839 eV  402.03 nm  f=0.0076
<S**2>=0.000
```

```
     322 -> 345        0.64949
     329 -> 346        0.15485
     340 -> 351       -0.11511
     341 -> 351        0.13041

 Excited State  88:      Singlet-A      3.0845 eV  401.95 nm  f=0.1160
<S**2>=0.000
     321 -> 345       -0.27748
     322 -> 345        0.15880
     323 -> 345        0.14016
     335 -> 348       -0.13318
     340 -> 351        0.53505
     341 -> 351       -0.15061

 Excited State  89:      Singlet-A      3.0863 eV  401.73 nm  f=0.0041
<S**2>=0.000
     321 -> 345        0.62946
     330 -> 347        0.10174
     340 -> 351        0.25787
     341 -> 351       -0.10635

 Excited State  90:      Singlet-A      3.0877 eV  401.54 nm  f=0.0014
<S**2>=0.000
     333 -> 348       -0.27138
     334 -> 348       -0.19029
     340 -> 351        0.20087
     341 -> 351        0.53437

 Excited State  91:      Singlet-A      3.0933 eV  400.81 nm  f=0.0747
<S**2>=0.000
     320 -> 345        0.10385
     330 -> 346        0.36864
     330 -> 347        0.48692
     332 -> 348       -0.16797
     340 -> 351       -0.10508

 Excited State  92:      Singlet-A      3.1081 eV  398.91 nm  f=0.0007
<S**2>=0.000
     322 -> 345       -0.13712
     329 -> 346        0.42927
     329 -> 347       -0.15705
     331 -> 346        0.18749
     332 -> 347        0.19082
     333 -> 348        0.10712
     344 -> 353       -0.32574
     344 -> 354        0.10555

 Excited State  93:      Singlet-A      3.1123 eV  398.36 nm  f=0.4001
<S**2>=0.000
     323 -> 345        0.19186
     328 -> 346       -0.14672
     330 -> 347       -0.12258
     338 -> 350       -0.17612
     340 -> 351       -0.13664
     342 -> 353       -0.18812
     343 -> 351        0.14353
     344 -> 352       -0.16939
     344 -> 353        0.16461
     344 -> 354        0.43948
```

```
 Excited State  94:      Singlet-A      3.1167 eV  397.81 nm  f=0.4358
<S**2>=0.000
     323 -> 345       -0.18725
     338 -> 350        0.18117
     340 -> 351        0.13972
     342 -> 353       -0.14172
     342 -> 354        0.13691
     343 -> 351       -0.14536
     344 -> 352        0.17404
     344 -> 354        0.43623

 Excited State  95:      Singlet-A      3.1167 eV  397.80 nm  f=0.0638
<S**2>=0.000
     322 -> 345       -0.10686
     329 -> 346        0.16523
     329 -> 347       -0.14449
     333 -> 348        0.14260
     334 -> 348        0.10070
     342 -> 353       -0.12766
     342 -> 354       -0.21310
     344 -> 353        0.49942

 Excited State  96:      Singlet-A      3.1219 eV  397.14 nm  f=0.0000
<S**2>=0.000
     329 -> 346        0.20011
     329 -> 347        0.39349
     330 -> 348       -0.12163
     331 -> 347        0.17419
     332 -> 346       -0.12702
     332 -> 347       -0.18721
     342 -> 352       -0.14934
     344 -> 355        0.34743

 Excited State  97:      Singlet-A      3.1291 eV  396.23 nm  f=0.0004
<S**2>=0.000
     343 -> 353        0.70034

 Excited State  98:      Singlet-A      3.1295 eV  396.17 nm  f=0.0000
<S**2>=0.000
     343 -> 354        0.70203

 Excited State  99:      Singlet-A      3.1329 eV  395.74 nm  f=0.0042
<S**2>=0.000
     328 -> 346       -0.10415
     329 -> 348       -0.23834
     331 -> 348        0.61946
     332 -> 348       -0.16083

 Excited State 100:      Singlet-A      3.1555 eV  392.91 nm  f=0.0404
<S**2>=0.000
     320 -> 345        0.11471
     325 -> 347       -0.14096
     328 -> 346       -0.22054
     329 -> 348       -0.31382
     330 -> 347        0.16545
     332 -> 348        0.43153
     343 -> 355       -0.25630
```

```
 Excited State 101:      Singlet-A      3.1654 eV  391.69 nm  f=0.0000
<S**2>=0.000
     319 -> 345        0.66407
     344 -> 355       -0.19843

 Excited State 102:      Singlet-A      3.1705 eV  391.05 nm  f=0.0388
<S**2>=0.000
     320 -> 345       -0.23947
     325 -> 346       -0.11833
     325 -> 347       -0.12797
     329 -> 348       -0.17157
     332 -> 348        0.16708
     343 -> 355        0.57547

 Excited State 103:      Singlet-A      3.1764 eV  390.33 nm  f=0.0058
<S**2>=0.000
     327 -> 348       -0.13122
     328 -> 346        0.45751
     328 -> 347       -0.16568
     329 -> 348       -0.37476
     342 -> 353       -0.15357
     343 -> 355       -0.13737

 Excited State 104:      Singlet-A      3.1809 eV  389.78 nm  f=0.0000
<S**2>=0.000
     327 -> 346        0.50110
     327 -> 347       -0.13547
     330 -> 348        0.36310
     342 -> 354        0.17244

 Excited State 105:      Singlet-A      3.1867 eV  389.07 nm  f=0.0137
<S**2>=0.000
     320 -> 345       -0.17027
     328 -> 346        0.24518
     328 -> 347        0.54952
     332 -> 348        0.19527
     342 -> 353       -0.11815
     343 -> 355       -0.10532

 Excited State 106:      Singlet-A      3.1897 eV  388.71 nm  f=0.0000
<S**2>=0.000
     317 -> 345        0.35874
     319 -> 345       -0.13154
     327 -> 346        0.22645
     327 -> 347        0.27900
     330 -> 348       -0.12805
     342 -> 352       -0.15028
     342 -> 354        0.11231
     344 -> 355       -0.34941

 Excited State 107:      Singlet-A      3.1961 eV  387.93 nm  f=0.0000
<S**2>=0.000
     317 -> 345       -0.19371
     318 -> 345       -0.24679
     326 -> 346        0.15849
     327 -> 347        0.52996
     328 -> 348        0.13109
     342 -> 354        0.12001
     344 -> 355        0.18121
```

```
 Excited State 108:      Singlet-A      3.2031 eV  387.07 nm  f=0.0000
<S**2>=0.000
     317 -> 345        0.12939
     318 -> 345        0.15095
     326 -> 346       -0.11657
     326 -> 347        0.18669
     327 -> 346       -0.27605
     327 -> 347        0.13547
     328 -> 348        0.31509
     330 -> 348        0.39764
     342 -> 354        0.11138

 Excited State 109:      Singlet-A      3.2047 eV  386.88 nm  f=0.0150
<S**2>=0.000
     320 -> 345       -0.15591
     325 -> 346       -0.19050
     327 -> 348        0.31840
     328 -> 346       -0.25180
     328 -> 347        0.19638
     329 -> 348       -0.21497
     330 -> 346        0.12209
     331 -> 348       -0.19787
     332 -> 348       -0.23818

 Excited State 110:      Singlet-A      3.2094 eV  386.31 nm  f=0.0023
<S**2>=0.000
     316 -> 345        0.63757
     320 -> 345       -0.17689
     328 -> 347       -0.11357

 Excited State 111:      Singlet-A      3.2134 eV  385.84 nm  f=0.0000
<S**2>=0.000
     317 -> 345       -0.16003
     318 -> 345        0.50794
     326 -> 346        0.36023
     326 -> 347        0.14702
     342 -> 354        0.13669

 Excited State 112:      Singlet-A      3.2177 eV  385.32 nm  f=0.0147
<S**2>=0.000
     312 -> 345        0.17961
     316 -> 345        0.27442
     320 -> 345        0.40754
     325 -> 346        0.15499
     325 -> 347        0.18472
     328 -> 347        0.11543
     329 -> 348       -0.13585
     341 -> 352        0.17740
     342 -> 353       -0.17941
     343 -> 355        0.16625

 Excited State 113:      Singlet-A      3.2214 eV  384.88 nm  f=0.0021
<S**2>=0.000
     320 -> 345       -0.11266
     325 -> 347       -0.17224
     341 -> 352        0.64814
```

```
 Excited State 114:      Singlet-A      3.2216 eV  384.85 nm  f=0.0032
<S**2>=0.000
     325 -> 346        0.46134
     325 -> 347       -0.37392
     326 -> 348       -0.24199
     341 -> 352       -0.19816
     342 -> 355       -0.14277

 Excited State 115:      Singlet-A      3.2226 eV  384.74 nm  f=0.0001
<S**2>=0.000
     340 -> 352        0.69849

 Excited State 116:      Singlet-A      3.2281 eV  384.08 nm  f=0.0000
<S**2>=0.000
     317 -> 345       -0.25423
     325 -> 348        0.29682
     326 -> 346       -0.37262
     326 -> 347        0.37535
     330 -> 348       -0.15009

 Excited State 117:      Singlet-A      3.2330 eV  383.50 nm  f=0.0075
<S**2>=0.000
     315 -> 345        0.69359

 Excited State 118:      Singlet-A      3.2427 eV  382.35 nm  f=0.0002
<S**2>=0.000
     317 -> 345        0.33694
     318 -> 345        0.20642
     319 -> 345        0.10356
     325 -> 348        0.10367
     326 -> 346       -0.12445
     326 -> 347       -0.10116
     327 -> 347        0.14155
     328 -> 348       -0.13825
     329 -> 347       -0.10789
     342 -> 352        0.15972
     342 -> 354       -0.13725
     343 -> 356       -0.26457
     344 -> 355        0.26489

 Excited State 119:      Singlet-A      3.2459 eV  381.97 nm  f=0.0840
<S**2>=0.000
     320 -> 345       -0.24858
     325 -> 346        0.25606
     325 -> 347        0.32477
     328 -> 346       -0.12349
     328 -> 347       -0.15341
     330 -> 347        0.11441
     332 -> 349        0.11183
     335 -> 349       -0.11481
     342 -> 353       -0.26687
     342 -> 354        0.12550
     344 -> 354       -0.10172

 Excited State 120:      Singlet-A      3.2475 eV  381.79 nm  f=0.0028
<S**2>=0.000
     317 -> 345        0.23487
     318 -> 345       -0.22765
     326 -> 346        0.19407
```

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     326 -> 347        0.34502
     327 -> 347       -0.13612
     330 -> 349       -0.11139
     342 -> 353        0.12355
     342 -> 354        0.20866
     344 -> 355        0.11560

 Excited State 121:      Singlet-A      3.2665 eV  379.56 nm  f=0.0866
<S**2>=0.000
     325 -> 347       -0.12585
     326 -> 348       -0.24809
     342 -> 355        0.60649

 Excited State 122:      Singlet-A      3.2887 eV  377.00 nm  f=0.0815
<S**2>=0.000
     325 -> 346        0.19082
     325 -> 347        0.24791
     333 -> 350       -0.16536
     334 -> 350       -0.15135
     342 -> 353        0.38123
     342 -> 354       -0.17818
     342 -> 355        0.14324
     344 -> 354        0.20935
     344 -> 356        0.17329

 Excited State 123:      Singlet-A      3.2889 eV  376.98 nm  f=0.0012
<S**2>=0.000
     326 -> 346       -0.19698
     326 -> 347       -0.26533
     335 -> 350        0.26220
     342 -> 353        0.17946
     342 -> 354        0.40044
     344 -> 353        0.20859

 Excited State 124:      Singlet-A      3.3153 eV  373.97 nm  f=0.0189
<S**2>=0.000
     324 -> 346        0.30819
     324 -> 347       -0.15041
     327 -> 348        0.35257
     330 -> 350       -0.12184
     333 -> 350       -0.11569
     334 -> 350       -0.21541
     335 -> 349       -0.12156
     344 -> 356       -0.33476

 Excited State 125:      Singlet-A      3.3175 eV  373.73 nm  f=0.0000
<S**2>=0.000
     327 -> 347       -0.11821
     328 -> 348        0.35217
     330 -> 348       -0.14198
     332 -> 350        0.17327
     333 -> 349        0.12078
     334 -> 349       -0.28450
     335 -> 350       -0.34732
     342 -> 354        0.10323

 Excited State 126:      Singlet-A      3.3197 eV  373.48 nm  f=0.0000
<S**2>=0.000
     328 -> 348        0.15747
```

```
     333 -> 349       -0.38184
     334 -> 349        0.50831
     335 -> 350       -0.16983

 Excited State 127:      Singlet-A      3.3213 eV  373.30 nm  f=0.0108
<S**2>=0.000
     324 -> 346       -0.26606
     324 -> 347        0.30072
     327 -> 348        0.32628
     330 -> 350       -0.13976
     333 -> 350       -0.15365
     334 -> 350       -0.12937
     344 -> 356        0.30540

 Excited State 128:      Singlet-A      3.3259 eV  372.78 nm  f=0.0009
<S**2>=0.000
     333 -> 350       -0.42893
     334 -> 350        0.54770

 Excited State 129:      Singlet-A      3.3399 eV  371.22 nm  f=0.0099
<S**2>=0.000
     311 -> 345       -0.10054
     325 -> 347        0.11239
     326 -> 348       -0.32375
     333 -> 350       -0.17942
     334 -> 350       -0.12754
     335 -> 349        0.49576

 Excited State 130:      Singlet-A      3.3429 eV  370.89 nm  f=0.0000
<S**2>=0.000
     325 -> 348       -0.28429
     327 -> 346       -0.12878
     328 -> 348       -0.27186
     333 -> 349        0.36026
     334 -> 349        0.23165
     335 -> 350       -0.30134

 Excited State 131:      Singlet-A      3.3484 eV  370.28 nm  f=0.0225
<S**2>=0.000
     311 -> 345        0.41668
     314 -> 345       -0.36091
     324 -> 346       -0.16393
     326 -> 348        0.15777
     333 -> 350       -0.19547
     334 -> 350       -0.13540
     335 -> 349        0.13453
     344 -> 357        0.14762

 Excited State 132:      Singlet-A      3.3533 eV  369.74 nm  f=0.0405
<S**2>=0.000
     311 -> 345        0.11348
     314 -> 345       -0.10585
     324 -> 346        0.30097
     327 -> 348        0.18484
     333 -> 350        0.28922
     334 -> 350        0.17799
     335 -> 349        0.30849
     344 -> 356        0.19777
     344 -> 357        0.19183
```

```
 Excited State 133:      Singlet-A      3.3559 eV  369.45 nm  f=0.0000
<S**2>=0.000
     325 -> 348       -0.23490
     326 -> 347        0.10545
     328 -> 348        0.23315
     332 -> 350        0.11332
     333 -> 349        0.28643
     334 -> 349        0.18304
     335 -> 350        0.37369

 Excited State 134:      Singlet-A      3.3664 eV  368.29 nm  f=0.0334
<S**2>=0.000
     324 -> 346        0.27020
     324 -> 347        0.52136
     326 -> 348        0.11075
     327 -> 348       -0.11187
     330 -> 350        0.11860
     332 -> 349        0.15520
     333 -> 350       -0.14553
     344 -> 356       -0.10407

 Excited State 135:      Singlet-A      3.3808 eV  366.73 nm  f=0.0003
<S**2>=0.000
     313 -> 345        0.10664
     323 -> 346        0.50626
     323 -> 347       -0.39017
     324 -> 348        0.14489
     325 -> 348        0.12056
     342 -> 356        0.13151

 Excited State 136:      Singlet-A      3.3814 eV  366.66 nm  f=0.0494
<S**2>=0.000
     312 -> 345        0.18098
     314 -> 345       -0.11998
     322 -> 346       -0.10319
     324 -> 346        0.30322
     324 -> 347       -0.13834
     325 -> 346       -0.12733
     326 -> 348       -0.11920
     327 -> 348       -0.13652
     329 -> 348        0.11139
     333 -> 350       -0.15885
     335 -> 349       -0.13445
     344 -> 356        0.30684

 Excited State 137:      Singlet-A      3.3883 eV  365.92 nm  f=0.0000
<S**2>=0.000
     323 -> 346       -0.14237
     324 -> 348       -0.13085
     325 -> 348        0.39847
     326 -> 346        0.16646
     326 -> 350        0.13575
     330 -> 349        0.10517
     333 -> 349        0.27768
     334 -> 349        0.19862
     340 -> 354       -0.10095
     341 -> 353        0.11034
     342 -> 357       -0.12197
```

```
 Excited State 138:      Singlet-A      3.3936 eV  365.35 nm  f=0.0363
<S**2>=0.000
     314 -> 345        0.22085
     324 -> 347       -0.18783
     325 -> 346        0.11553
     325 -> 347       -0.11455
     325 -> 350        0.12705
     326 -> 348        0.35206
     330 -> 350        0.14089
     331 -> 349        0.10951
     332 -> 349       -0.22873
     333 -> 350       -0.16206
     334 -> 350       -0.12375
     335 -> 349        0.11015
     344 -> 356        0.13855

 Excited State 139:      Singlet-A      3.4009 eV  364.56 nm  f=0.0000
<S**2>=0.000
     324 -> 348       -0.13868
     340 -> 354       -0.21602
     341 -> 353       -0.40471
     341 -> 354        0.42342
     342 -> 356       -0.25557

 Excited State 140:      Singlet-A      3.4012 eV  364.53 nm  f=0.0001
<S**2>=0.000
     324 -> 348        0.12931
     340 -> 353        0.39766
     341 -> 353        0.25543
     341 -> 354        0.42791
     342 -> 356        0.23052

 Excited State 141:      Singlet-A      3.4015 eV  364.50 nm  f=0.0000
<S**2>=0.000
     324 -> 348       -0.20422
     332 -> 350        0.14442
     340 -> 353        0.27376
     340 -> 354        0.37081
     341 -> 353        0.21664
     342 -> 356       -0.36986

 Excited State 142:      Singlet-A      3.4057 eV  364.05 nm  f=0.0109
<S**2>=0.000
     313 -> 345       -0.21799
     340 -> 353        0.44578
     341 -> 353       -0.35675
     341 -> 354       -0.27407
     342 -> 356        0.10811

 Excited State 143:      Singlet-A      3.4061 eV  364.01 nm  f=0.0027
<S**2>=0.000
     313 -> 345        0.57334
     314 -> 346       -0.13003
     314 -> 347        0.10532
     332 -> 350       -0.13664
     340 -> 353        0.19011
     341 -> 354       -0.13651
```

```
 Excited State 144:      Singlet-A      3.4076 eV  363.84 nm  f=0.0040
<S**2>=0.000
     340 -> 353       -0.13590
     340 -> 354        0.53509
     341 -> 353       -0.26336
     341 -> 354        0.18433
     342 -> 356        0.12615

 Excited State 145:      Singlet-A      3.4121 eV  363.36 nm  f=0.0000
<S**2>=0.000
     323 -> 346        0.41245
     323 -> 347        0.52284

 Excited State 146:      Singlet-A      3.4158 eV  362.97 nm  f=0.0866
<S**2>=0.000
     312 -> 345        0.50287
     314 -> 345        0.11666
     320 -> 345       -0.12292
     331 -> 349        0.29666
     332 -> 349        0.12947
     344 -> 356       -0.11698

 Excited State 147:      Singlet-A      3.4201 eV  362.51 nm  f=0.0236
<S**2>=0.000
     311 -> 345        0.42194
     313 -> 346       -0.13882
     313 -> 347        0.11561
     314 -> 345        0.43280
     329 -> 349        0.13011
     331 -> 349       -0.20939

 Excited State 148:      Singlet-A      3.4254 eV  361.96 nm  f=0.0059
<S**2>=0.000
     311 -> 345        0.12336
     312 -> 345       -0.13281
     329 -> 349       -0.25348
     329 -> 350        0.13888
     331 -> 349        0.35756
     331 -> 350       -0.27209
     332 -> 350        0.26054
     339 -> 351        0.10037

 Excited State 149:      Singlet-A      3.4256 eV  361.94 nm  f=0.0052
<S**2>=0.000
     311 -> 345        0.12092
     312 -> 345       -0.12775
     329 -> 349       -0.22486
     329 -> 350       -0.16980
     331 -> 349        0.30150
     331 -> 350        0.31369
     332 -> 350       -0.28432
     339 -> 351       -0.10887

 Excited State 150:      Singlet-A      3.4333 eV  361.12 nm  f=0.0007
<S**2>=0.000
     341 -> 355        0.69060

 Excited State 151:      Singlet-A      3.4345 eV  361.00 nm  f=0.0027
<S**2>=0.000
```

```
     340 -> 355        0.68431

 Excited State 152:      Singlet-A      3.4364 eV  360.80 nm  f=0.0000
<S**2>=0.000
     329 -> 350       -0.24402
     331 -> 350        0.40173
     332 -> 350        0.33654
     339 -> 351        0.18855
     342 -> 356        0.11393
     343 -> 356       -0.13104

 Excited State 153:      Singlet-A      3.4423 eV  360.17 nm  f=0.0178
<S**2>=0.000
     321 -> 348        0.16158
     322 -> 346        0.62345
     329 -> 349       -0.10763
     344 -> 357       -0.16146

 Excited State 154:      Singlet-A      3.4427 eV  360.14 nm  f=0.0000
<S**2>=0.000
     324 -> 348        0.51242
     342 -> 356       -0.22527
     343 -> 356       -0.13505
     343 -> 357        0.27909

 Excited State 155:      Singlet-A      3.4442 eV  359.98 nm  f=0.0000
<S**2>=0.000
     321 -> 346        0.63629
     322 -> 348        0.19194
     343 -> 356        0.12091

 Excited State 156:      Singlet-A      3.4493 eV  359.45 nm  f=0.0001
<S**2>=0.000
     312 -> 345        0.10799
     321 -> 348       -0.11824
     322 -> 347        0.57805
     330 -> 350       -0.16823
     331 -> 349       -0.11031
     332 -> 349       -0.19949

 Excited State 157:      Singlet-A      3.4505 eV  359.32 nm  f=0.0001
<S**2>=0.000
     321 -> 347        0.42750
     324 -> 348        0.11822
     329 -> 350       -0.31021
     330 -> 349       -0.12262
     331 -> 350       -0.14237
     339 -> 351        0.34091
     343 -> 356        0.11134

 Excited State 158:      Singlet-A      3.4520 eV  359.17 nm  f=0.0018
<S**2>=0.000
     310 -> 345        0.68291

 Excited State 159:      Singlet-A      3.4529 eV  359.07 nm  f=0.0423
<S**2>=0.000
     310 -> 345        0.11786
     312 -> 345       -0.11882
     322 -> 346        0.16020
```

```
     322 -> 347        0.26721
     323 -> 348       -0.15447
     329 -> 349        0.20106
     330 -> 350        0.33396
     331 -> 349        0.16670
     332 -> 349        0.11007
     344 -> 357        0.27509

 Excited State 160:      Singlet-A      3.4536 eV  359.00 nm  f=0.0000
<S**2>=0.000
     307 -> 345        0.21758
     320 -> 346       -0.18307
     320 -> 347        0.14628
     321 -> 346       -0.13488
     321 -> 347       -0.26060
     324 -> 348        0.15175
     332 -> 350        0.10168
     338 -> 351        0.10289
     342 -> 356       -0.11745
     343 -> 356        0.39439

 Excited State 161:      Singlet-A      3.4576 eV  358.59 nm  f=0.0000
<S**2>=0.000
     320 -> 347        0.13705
     321 -> 347        0.34527
     329 -> 350        0.30589
     330 -> 349       -0.23112
     331 -> 350        0.18209
     332 -> 350        0.19884
     339 -> 351       -0.23832
     343 -> 357       -0.12785

 Excited State 162:      Singlet-A      3.4613 eV  358.20 nm  f=0.0127
<S**2>=0.000
     312 -> 345       -0.12006
     318 -> 347        0.10932
     319 -> 347        0.10851
     321 -> 348       -0.10372
     322 -> 347        0.13282
     324 -> 347       -0.10635
     325 -> 350        0.11362
     326 -> 348        0.11856
     330 -> 350       -0.20636
     332 -> 349        0.48812
     335 -> 349        0.10693

 Excited State 163:      Singlet-A      3.4673 eV  357.58 nm  f=0.0000
<S**2>=0.000
     320 -> 346       -0.10495
     321 -> 347        0.15075
     330 -> 349        0.52341
     339 -> 351       -0.11991
     342 -> 357        0.10099
     343 -> 356        0.10742
     343 -> 357       -0.27510

 Excited State 164:      Singlet-A      3.4686 eV  357.44 nm  f=0.0000
<S**2>=0.000
     321 -> 347        0.14551
```

```
     324 -> 348       -0.18446
     330 -> 349        0.16457
     342 -> 356        0.22375
     343 -> 357        0.53593

 Excited State 165:      Singlet-A      3.4688 eV  357.42 nm  f=0.0001
<S**2>=0.000
     309 -> 345        0.70043

 Excited State 166:      Singlet-A      3.4714 eV  357.16 nm  f=0.0105
<S**2>=0.000
     308 -> 345        0.47669
     328 -> 350       -0.14734
     329 -> 349        0.26248
     330 -> 350       -0.28133
     331 -> 349        0.14334
     344 -> 357        0.11569

 Excited State 167:      Singlet-A      3.4715 eV  357.15 nm  f=0.0092
<S**2>=0.000
     308 -> 345        0.51125
     328 -> 350        0.13637
     329 -> 349       -0.24419
     330 -> 350        0.25856
     331 -> 349       -0.13582
     344 -> 357       -0.10858

 Excited State 168:      Singlet-A      3.4775 eV  356.53 nm  f=0.0062
<S**2>=0.000
     322 -> 346        0.11446
     322 -> 347        0.10120
     323 -> 348        0.66356

 Excited State 169:      Singlet-A      3.5034 eV  353.90 nm  f=0.0740
<S**2>=0.000
     318 -> 346       -0.12580
     319 -> 346        0.49490
     319 -> 347        0.19075
     321 -> 348        0.16054
     328 -> 350       -0.16042
     329 -> 349       -0.15366
     339 -> 352       -0.13953
     344 -> 357        0.26199

 Excited State 170:      Singlet-A      3.5101 eV  353.22 nm  f=0.0293
<S**2>=0.000
     317 -> 346       -0.20590
     319 -> 346        0.43967
     319 -> 347       -0.32794
     321 -> 348       -0.11821
     329 -> 349        0.17761
     339 -> 352        0.15574
     344 -> 357       -0.20432

 Excited State 171:      Singlet-A      3.5165 eV  352.58 nm  f=0.0084
<S**2>=0.000
     317 -> 346       -0.10990
     317 -> 347       -0.18312
     318 -> 347       -0.13770
```

```
     319 -> 347        0.54481
     329 -> 349        0.18030
     339 -> 352        0.17099
     344 -> 357       -0.17112

 Excited State 172:      Singlet-A      3.5307 eV  351.16 nm  f=0.0000
<S**2>=0.000
     320 -> 346       -0.15903
     327 -> 350        0.11113
     328 -> 349       -0.17406
     329 -> 350        0.32789
     331 -> 350        0.14029
     332 -> 350       -0.15578
     339 -> 351        0.44005

 Excited State 173:      Singlet-A      3.5358 eV  350.65 nm  f=0.0000
<S**2>=0.000
     307 -> 345        0.17750
     320 -> 346        0.18466
     320 -> 347       -0.12690
     322 -> 348        0.25714
     326 -> 350        0.17860
     338 -> 351        0.12034
     342 -> 357        0.49532

 Excited State 174:      Singlet-A      3.5478 eV  349.46 nm  f=0.0000
<S**2>=0.000
     316 -> 346        0.55071
     320 -> 346       -0.17459
     327 -> 350        0.25486
     342 -> 357        0.20966

 Excited State 175:      Singlet-A      3.5505 eV  349.20 nm  f=0.0000
<S**2>=0.000
     316 -> 346        0.21025
     316 -> 347        0.37534
     318 -> 348       -0.10435
     320 -> 347       -0.25947
     327 -> 350       -0.22964
     328 -> 349       -0.36397
     342 -> 357       -0.10231

 Excited State 176:      Singlet-A      3.5543 eV  348.83 nm  f=0.0063
<S**2>=0.000
     317 -> 347       -0.14363
     318 -> 346       -0.30969
     318 -> 347        0.16352
     320 -> 348        0.11073
     321 -> 348        0.16839
     328 -> 350        0.50483

 Excited State 177:      Singlet-A      3.5557 eV  348.69 nm  f=0.0001
<S**2>=0.000
     307 -> 345        0.14052
     316 -> 346        0.34042
     318 -> 348       -0.18538
     320 -> 346        0.23270
     322 -> 348       -0.13360
     327 -> 350       -0.20130
```

```
     328 -> 349        0.34785
     329 -> 350        0.10231
     342 -> 357       -0.10837

 Excited State 178:      Singlet-A      3.5585 eV  348.41 nm  f=0.0165
<S**2>=0.000
     317 -> 347        0.17590
     318 -> 346        0.28014
     320 -> 348       -0.22946
     321 -> 348        0.45637
     322 -> 347        0.10270
     327 -> 349        0.17830
     328 -> 350        0.15902
     339 -> 352        0.10574

 Excited State 179:      Singlet-A      3.5598 eV  348.29 nm  f=0.0001
<S**2>=0.000
     316 -> 347        0.55903
     328 -> 349        0.35756

 Excited State 180:      Singlet-A      3.5644 eV  347.84 nm  f=0.0035
<S**2>=0.000
     317 -> 347       -0.10015
     318 -> 347        0.17186
     320 -> 348        0.17896
     322 -> 348        0.22618
     327 -> 349        0.50650
     327 -> 350       -0.17036

 Excited State 181:      Singlet-A      3.5646 eV  347.82 nm  f=0.0014
<S**2>=0.000
     315 -> 346        0.12201
     316 -> 347       -0.10810
     318 -> 347       -0.11320
     318 -> 348        0.15299
     320 -> 346       -0.11876
     320 -> 347        0.11027
     320 -> 348       -0.10668
     322 -> 348        0.36227
     326 -> 350       -0.11046
     327 -> 349       -0.30009
     327 -> 350       -0.31106

 Excited State 182:      Singlet-A      3.5699 eV  347.30 nm  f=0.0157
<S**2>=0.000
     317 -> 346        0.16985
     317 -> 347        0.23279
     318 -> 346       -0.11089
     318 -> 347        0.23176
     320 -> 348        0.31012
     321 -> 348        0.19218
     327 -> 349       -0.19710
     328 -> 350       -0.21251
     339 -> 352        0.24292
     344 -> 357       -0.13247

 Excited State 183:      Singlet-A      3.5737 eV  346.94 nm  f=0.0045
<S**2>=0.000
     317 -> 346        0.36413
```

```
     317 -> 347       -0.20411
     318 -> 347       -0.18791
     326 -> 349        0.31750
     341 -> 356        0.38295

 Excited State 184:      Singlet-A      3.5749 eV  346.82 nm  f=0.0002
<S**2>=0.000
     315 -> 346        0.65506
     315 -> 347       -0.10853
     327 -> 350        0.10359
     341 -> 356        0.14013

 Excited State 185:      Singlet-A      3.5762 eV  346.70 nm  f=0.0002
<S**2>=0.000
     307 -> 345       -0.10668
     340 -> 356        0.68391

 Excited State 186:      Singlet-A      3.5764 eV  346.67 nm  f=0.0091
<S**2>=0.000
     317 -> 346       -0.26226
     318 -> 347        0.13760
     326 -> 349       -0.19617
     327 -> 349        0.10704
     341 -> 356        0.56571

 Excited State 187:      Singlet-A      3.5825 eV  346.08 nm  f=0.0000
<S**2>=0.000
     315 -> 347        0.64440
     326 -> 350       -0.11989
     327 -> 350        0.16113

 Excited State 188:      Singlet-A      3.5862 eV  345.72 nm  f=0.0000
<S**2>=0.000
     319 -> 348        0.55772
     320 -> 347       -0.15131
     325 -> 349        0.33982

 Excited State 189:      Singlet-A      3.5905 eV  345.31 nm  f=0.0001
<S**2>=0.000
     307 -> 345       -0.17868
     315 -> 347        0.18633
     317 -> 348       -0.10750
     318 -> 348        0.17359
     319 -> 348        0.15272
     322 -> 348       -0.26725
     326 -> 350        0.28516
     327 -> 350       -0.28495
     338 -> 351        0.18905
     342 -> 357        0.14769

 Excited State 190:      Singlet-A      3.5937 eV  345.01 nm  f=0.0001
<S**2>=0.000
     307 -> 345        0.43708
     312 -> 346       -0.10318
     318 -> 348        0.17762
     326 -> 350        0.28513
     338 -> 351       -0.28494
     343 -> 356       -0.12183
```

```
 Excited State 191:      Singlet-A      3.5954 eV  344.84 nm  f=0.0566
<S**2>=0.000
     317 -> 346       -0.18122
     317 -> 347       -0.17962
     318 -> 347       -0.10520
     320 -> 348        0.13132
     321 -> 348        0.17137
     325 -> 350        0.53153
     339 -> 352       -0.21501

 Excited State 192:      Singlet-A      3.5980 eV  344.59 nm  f=0.0000
<S**2>=0.000
     317 -> 348        0.22296
     318 -> 348        0.11324
     319 -> 348       -0.35838
     320 -> 346       -0.13592
     320 -> 347       -0.17901
     325 -> 349        0.43274

 Excited State 193:      Singlet-A      3.6127 eV  343.19 nm  f=0.0421
<S**2>=0.000
     314 -> 348        0.10607
     317 -> 346       -0.22029
     317 -> 347        0.30471
     318 -> 346       -0.18527
     326 -> 349        0.46778

 Excited State 194:      Singlet-A      3.6257 eV  341.96 nm  f=0.0000
<S**2>=0.000
     314 -> 346        0.46428
     314 -> 347        0.48389

 Excited State 195:      Singlet-A      3.6281 eV  341.73 nm  f=0.0004
<S**2>=0.000
     313 -> 346        0.48327
     313 -> 347        0.49950

 Excited State 196:      Singlet-A      3.6345 eV  341.13 nm  f=0.0077
<S**2>=0.000
     316 -> 348        0.61898
     317 -> 347       -0.13503
     320 -> 348       -0.10378
     325 -> 350       -0.11536
     328 -> 350       -0.12686

 Excited State 197:      Singlet-A      3.6397 eV  340.64 nm  f=0.0257
<S**2>=0.000
     316 -> 348        0.32774
     317 -> 346        0.17125
     317 -> 347        0.24978
     318 -> 346        0.10176
     321 -> 348       -0.22495
     322 -> 350        0.11532
     325 -> 350        0.24091
     328 -> 350        0.17328
     339 -> 352       -0.13903

 Excited State 198:      Singlet-A      3.6443 eV  340.22 nm  f=0.0000
<S**2>=0.000
```

```
     307 -> 345       -0.20103
     312 -> 346        0.21882
     312 -> 347       -0.16012
     318 -> 348       -0.10102
     322 -> 348        0.16498
     325 -> 348       -0.13060
     326 -> 350        0.41984
     327 -> 350        0.10737
     342 -> 357       -0.18232

 Excited State 199:      Singlet-A      3.6529 eV  339.41 nm  f=0.0000
<S**2>=0.000
     311 -> 346        0.12898
     312 -> 346        0.10192
     314 -> 346       -0.25275
     314 -> 347        0.26721
     317 -> 348        0.45078
     318 -> 348        0.13673
     325 -> 349       -0.19364

 Excited State 200:      Singlet-A      3.6581 eV  338.93 nm  f=0.0012
<S**2>=0.000
     315 -> 348        0.70343
```

4a – CH_2Cl_2 BP86/6-31+G(d)

```
Excited State   1:      Singlet-A      1.3196 eV  939.58 nm  f=0.0124
<S**2>=0.000
     342 -> 346       -0.11566
     343 -> 347       -0.14569
     344 -> 345        0.67244
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4240.58805671
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      1.3290 eV  932.92 nm  f=0.3958
<S**2>=0.000
     343 -> 345        0.68238
     344 -> 347       -0.15950

 Excited State   3:      Singlet-A      1.5747 eV  787.33 nm  f=0.1412
<S**2>=0.000
     340 -> 345       -0.25946
     342 -> 345        0.47534
     343 -> 348       -0.13643
     344 -> 346       -0.37022
     344 -> 347        0.18366
     344 -> 349        0.10323

 Excited State   4:      Singlet-A      1.5928 eV  778.42 nm  f=0.0000
<S**2>=0.000
     341 -> 345        0.70694
```

```
 Excited State   5:      Singlet-A      1.5965 eV  776.62 nm  f=0.0212
<S**2>=0.000
     340 -> 345        0.65559
     342 -> 345        0.15011
     344 -> 346       -0.17886

 Excited State   6:      Singlet-A      1.6754 eV  740.04 nm  f=0.0000
<S**2>=0.000
     343 -> 346        0.51184
     343 -> 347       -0.25035
     344 -> 348        0.41192

 Excited State   7:      Singlet-A      1.7145 eV  723.13 nm  f=0.1476
<S**2>=0.000
     342 -> 345        0.41826
     342 -> 350        0.16668
     343 -> 348        0.29235
     344 -> 346        0.40072
     344 -> 347       -0.14397
     344 -> 349        0.15236

 Excited State   8:      Singlet-A      1.7297 eV  716.78 nm  f=0.8441
<S**2>=0.000
     342 -> 348        0.12420
     343 -> 345        0.15280
     343 -> 350       -0.22700
     344 -> 346        0.25231
     344 -> 347        0.58454

 Excited State   9:      Singlet-A      1.7461 eV  710.06 nm  f=0.0000
<S**2>=0.000
     342 -> 346        0.36696
     342 -> 347        0.58853
     344 -> 348       -0.10755

 Excited State  10:      Singlet-A      1.7631 eV  703.21 nm  f=0.0036
<S**2>=0.000
     339 -> 345       -0.18998
     342 -> 346        0.40388
     342 -> 347       -0.28083
     343 -> 346       -0.17260
     343 -> 347       -0.36694
     344 -> 350        0.22299

 Excited State  11:      Singlet-A      1.8509 eV  669.85 nm  f=0.0244
<S**2>=0.000
     339 -> 345       -0.18523
     342 -> 346        0.34567
     342 -> 347       -0.19696
     342 -> 349        0.11801
     343 -> 346        0.18604
     343 -> 347        0.36577
     344 -> 345        0.14856
     344 -> 350       -0.31687

 Excited State  12:      Singlet-A      1.8589 eV  666.96 nm  f=0.2633
<S**2>=0.000
     342 -> 348        0.69389
```

```
 Excited State  13:      Singlet-A      1.8933 eV  654.85 nm  f=0.0000
<S**2>=0.000
     343 -> 346       -0.28866
     343 -> 347        0.14776
     343 -> 349        0.42130
     344 -> 348        0.44575

 Excited State  14:      Singlet-A      1.9188 eV  646.16 nm  f=0.0024
<S**2>=0.000
     342 -> 345       -0.13518
     342 -> 350       -0.24868
     343 -> 348        0.40137
     344 -> 346       -0.18304
     344 -> 349        0.46053

 Excited State  15:      Singlet-A      1.9854 eV  624.48 nm  f=0.0016
<S**2>=0.000
     341 -> 346        0.70229

 Excited State  16:      Singlet-A      1.9856 eV  624.41 nm  f=0.0001
<S**2>=0.000
     339 -> 345       -0.17679
     340 -> 346        0.65913
     342 -> 349       -0.10911

 Excited State  17:      Singlet-A      1.9922 eV  622.35 nm  f=0.0011
<S**2>=0.000
     341 -> 347        0.70315

 Excited State  18:      Singlet-A      1.9927 eV  622.18 nm  f=0.0014
<S**2>=0.000
     339 -> 345        0.30812
     340 -> 346        0.22202
     340 -> 347        0.52263
     342 -> 349        0.24570

 Excited State  19:      Singlet-A      1.9948 eV  621.54 nm  f=0.0034
<S**2>=0.000
     339 -> 345       -0.37620
     340 -> 346       -0.11037
     340 -> 347        0.46327
     342 -> 349       -0.31328
     344 -> 350       -0.12338

 Excited State  20:      Singlet-A      2.1059 eV  588.75 nm  f=0.0017
<S**2>=0.000
     341 -> 348        0.69666

 Excited State  21:      Singlet-A      2.1075 eV  588.31 nm  f=0.0004
<S**2>=0.000
     340 -> 348        0.70456

 Excited State  22:      Singlet-A      2.1365 eV  580.32 nm  f=0.0569
<S**2>=0.000
     338 -> 345       -0.27456
     341 -> 348        0.10676
     342 -> 349       -0.31826
     343 -> 346        0.12921
     343 -> 347        0.24850
```

```
     344 -> 345        0.12250
     344 -> 350        0.43134

 Excited State  23:      Singlet-A      2.1424 eV  578.70 nm  f=0.0142
<S**2>=0.000
     338 -> 345        0.62646
     342 -> 349       -0.14801
     343 -> 347        0.10443
     343 -> 349        0.11968
     344 -> 350        0.18274

 Excited State  24:      Singlet-A      2.1610 eV  573.75 nm  f=0.3695
<S**2>=0.000
     339 -> 346        0.30814
     339 -> 347       -0.10425
     343 -> 348       -0.38193
     344 -> 346        0.16040
     344 -> 349        0.42878

 Excited State  25:      Singlet-A      2.1768 eV  569.58 nm  f=0.5352
<S**2>=0.000
     339 -> 347        0.27093
     343 -> 350        0.59379
     344 -> 347        0.17311

 Excited State  26:      Singlet-A      2.1939 eV  565.13 nm  f=0.0272
<S**2>=0.000
     337 -> 345        0.14824
     339 -> 346        0.15394
     339 -> 349       -0.12208
     342 -> 345       -0.15992
     342 -> 350        0.58135
     343 -> 348        0.18574
     344 -> 346       -0.15139

 Excited State  27:      Singlet-A      2.1968 eV  564.39 nm  f=0.0010
<S**2>=0.000
     336 -> 345       -0.12213
     338 -> 345       -0.10279
     339 -> 348       -0.23781
     343 -> 346        0.19150
     343 -> 347       -0.11573
     343 -> 349        0.51255
     344 -> 348       -0.29508

 Excited State  28:      Singlet-A      2.2124 eV  560.40 nm  f=0.0184
<S**2>=0.000
     337 -> 345        0.68594
     342 -> 350       -0.11963

 Excited State  29:      Singlet-A      2.2238 eV  557.54 nm  f=0.0012
<S**2>=0.000
     336 -> 345        0.68718
     338 -> 345       -0.11162

 Excited State  30:      Singlet-A      2.3307 eV  531.96 nm  f=0.0039
<S**2>=0.000
     341 -> 349        0.70555
```

```
 Excited State  31:      Singlet-A      2.3310 eV  531.89 nm  f=0.0004
<S**2>=0.000
     340 -> 349        0.70382

 Excited State  32:      Singlet-A      2.3432 eV  529.13 nm  f=0.0000
<S**2>=0.000
     341 -> 350        0.70553

 Excited State  33:      Singlet-A      2.3448 eV  528.77 nm  f=0.0004
<S**2>=0.000
     340 -> 350        0.70492

 Excited State  34:      Singlet-A      2.4323 eV  509.74 nm  f=0.1332
<S**2>=0.000
     338 -> 346       -0.15564
     339 -> 346        0.29340
     339 -> 347        0.52704
     343 -> 350       -0.21368

 Excited State  35:      Singlet-A      2.4929 eV  497.35 nm  f=0.1501
<S**2>=0.000
     335 -> 345        0.58871
     338 -> 347       -0.11239
     339 -> 346        0.22706
     339 -> 347       -0.17424
     344 -> 349       -0.10025

 Excited State  36:      Singlet-A      2.4995 eV  496.04 nm  f=0.0016
<S**2>=0.000
     334 -> 345        0.70075

 Excited State  37:      Singlet-A      2.5049 eV  494.97 nm  f=0.4358
<S**2>=0.000
     333 -> 345        0.16498
     335 -> 345       -0.35840
     339 -> 346        0.41144
     339 -> 347       -0.20013
     339 -> 349        0.18376
     342 -> 350       -0.13324
     343 -> 348        0.12463
     344 -> 349       -0.17232

 Excited State  38:      Singlet-A      2.5160 eV  492.78 nm  f=0.0000
<S**2>=0.000
     332 -> 345       -0.11036
     339 -> 348        0.64282
     343 -> 349        0.14302
     344 -> 348       -0.12536

 Excited State  39:      Singlet-A      2.5461 eV  486.95 nm  f=0.3115
<S**2>=0.000
     330 -> 345       -0.13496
     331 -> 345       -0.10473
     336 -> 346        0.12647
     338 -> 346        0.61126
     338 -> 347       -0.18557
     339 -> 347        0.10316
```

```
 Excited State  40:      Singlet-A      2.5574 eV  484.81 nm  f=0.0106
<S**2>=0.000
     338 -> 348        0.10622
     339 -> 345       -0.32842
     339 -> 350       -0.28374
     342 -> 346       -0.16613
     342 -> 349        0.34943
     343 -> 347        0.12434
     344 -> 350        0.25373

 Excited State  41:      Singlet-A      2.5786 eV  480.81 nm  f=0.1226
<S**2>=0.000
     336 -> 346        0.16936
     336 -> 347        0.26329
     338 -> 346        0.17516
     338 -> 347        0.58484

 Excited State  42:      Singlet-A      2.6008 eV  476.72 nm  f=0.0848
<S**2>=0.000
     333 -> 345        0.66211
     336 -> 346       -0.10708

 Excited State  43:      Singlet-A      2.6032 eV  476.28 nm  f=0.0001
<S**2>=0.000
     332 -> 345        0.16363
     337 -> 346        0.67484

 Excited State  44:      Singlet-A      2.6108 eV  474.88 nm  f=0.0020
<S**2>=0.000
     332 -> 345        0.25432
     337 -> 347        0.65252

 Excited State  45:      Singlet-A      2.6151 eV  474.12 nm  f=0.0001
<S**2>=0.000
     332 -> 345        0.62182
     337 -> 346       -0.15497
     337 -> 347       -0.25738

 Excited State  46:      Singlet-A      2.6161 eV  473.93 nm  f=0.0723
<S**2>=0.000
     333 -> 345        0.11101
     336 -> 346        0.60900
     336 -> 347       -0.30235

 Excited State  47:      Singlet-A      2.6343 eV  470.66 nm  f=0.0896
<S**2>=0.000
     336 -> 346        0.24858
     336 -> 347        0.57616
     338 -> 346       -0.12637
     338 -> 347       -0.27295

 Excited State  48:      Singlet-A      2.6488 eV  468.07 nm  f=0.0064
<S**2>=0.000
     338 -> 348        0.67906
     339 -> 350        0.10050

 Excited State  49:      Singlet-A      2.6656 eV  465.12 nm  f=0.0025
<S**2>=0.000
     330 -> 345       -0.33643
```

```
     331 -> 345        0.61964

 Excited State  50:      Singlet-A      2.7173 eV  456.28 nm  f=0.0735
<S**2>=0.000
     330 -> 345        0.55398
     331 -> 345        0.27593
     337 -> 348       -0.12663
     338 -> 349        0.19611
     342 -> 351       -0.14308

 Excited State  51:      Singlet-A      2.7252 eV  454.96 nm  f=0.0031
<S**2>=0.000
     328 -> 345       -0.13292
     330 -> 345        0.10267
     337 -> 348        0.68024

 Excited State  52:      Singlet-A      2.7282 eV  454.45 nm  f=0.0002
<S**2>=0.000
     329 -> 345        0.63905
     336 -> 348       -0.27113

 Excited State  53:      Singlet-A      2.7355 eV  453.24 nm  f=0.0007
<S**2>=0.000
     329 -> 345        0.25378
     336 -> 348        0.64579

 Excited State  54:      Singlet-A      2.7375 eV  452.91 nm  f=0.0966
<S**2>=0.000
     328 -> 345        0.67619
     337 -> 348        0.13849

 Excited State  55:      Singlet-A      2.7637 eV  448.61 nm  f=0.0001
<S**2>=0.000
     327 -> 345        0.68972
     344 -> 351       -0.10519

 Excited State  56:      Singlet-A      2.8004 eV  442.74 nm  f=0.0371
<S**2>=0.000
     326 -> 345        0.67053
     339 -> 349       -0.19268

 Excited State  57:      Singlet-A      2.8100 eV  441.22 nm  f=0.0007
<S**2>=0.000
     324 -> 345       -0.15711
     325 -> 345        0.27503
     339 -> 345       -0.12677
     339 -> 350        0.50282
     342 -> 349        0.14313
     344 -> 351        0.24611

 Excited State  58:      Singlet-A      2.8137 eV  440.65 nm  f=0.0003
<S**2>=0.000
     338 -> 350        0.11359
     339 -> 350       -0.25046
     344 -> 351        0.59388

 Excited State  59:      Singlet-A      2.8248 eV  438.91 nm  f=0.0002
<S**2>=0.000
     325 -> 345        0.64552
```

```
     339 -> 350       -0.18698
     344 -> 351       -0.13114

 Excited State  60:      Singlet-A      2.8459 eV  435.66 nm  f=0.0722
<S**2>=0.000
     314 -> 345        0.11555
     326 -> 345        0.20125
     339 -> 346       -0.13413
     339 -> 349        0.59380
     342 -> 350        0.11652

 Excited State  61:      Singlet-A      2.8679 eV  432.32 nm  f=0.0001
<S**2>=0.000
     338 -> 350        0.68656
     344 -> 351       -0.11417

 Excited State  62:      Singlet-A      2.8837 eV  429.95 nm  f=0.0734
<S**2>=0.000
     343 -> 351        0.66615

 Excited State  63:      Singlet-A      2.8914 eV  428.80 nm  f=0.0051
<S**2>=0.000
     334 -> 346        0.16421
     336 -> 349        0.11041
     338 -> 349        0.48280
     342 -> 351        0.43796
     343 -> 351       -0.12533

 Excited State  64:      Singlet-A      2.8942 eV  428.39 nm  f=0.0003
<S**2>=0.000
     334 -> 348       -0.16037
     335 -> 346        0.63332
     335 -> 347       -0.25512

 Excited State  65:      Singlet-A      2.8980 eV  427.83 nm  f=0.0076
<S**2>=0.000
     334 -> 346        0.60585
     334 -> 347       -0.23335
     335 -> 348       -0.16485
     338 -> 349       -0.11066
     342 -> 351       -0.16949

 Excited State  66:      Singlet-A      2.9267 eV  423.63 nm  f=0.0061
<S**2>=0.000
     335 -> 346        0.25531
     335 -> 347        0.63271

 Excited State  67:      Singlet-A      2.9271 eV  423.58 nm  f=0.0338
<S**2>=0.000
     334 -> 346        0.20072
     334 -> 347        0.57160
     336 -> 349        0.12760
     338 -> 349        0.15136
     342 -> 351       -0.16038
     344 -> 352       -0.20641

 Excited State  68:      Singlet-A      2.9360 eV  422.30 nm  f=0.0691
<S**2>=0.000
     334 -> 346        0.15590
```

```
     334 -> 347        0.27518
     336 -> 349       -0.26526
     338 -> 349       -0.21230
     342 -> 351        0.30338
     344 -> 352        0.39964

 Excited State  69:      Singlet-A      2.9489 eV  420.44 nm  f=0.0000
<S**2>=0.000
     337 -> 349        0.70206

 Excited State  70:      Singlet-A      2.9615 eV  418.65 nm  f=0.0089
<S**2>=0.000
     334 -> 347        0.10542
     337 -> 350        0.68739

 Excited State  71:      Singlet-A      2.9638 eV  418.32 nm  f=0.0002
<S**2>=0.000
     336 -> 349        0.60668
     338 -> 349       -0.12307
     344 -> 352        0.31379

 Excited State  72:      Singlet-A      2.9709 eV  417.32 nm  f=0.0004
<S**2>=0.000
     336 -> 350        0.69621

 Excited State  73:      Singlet-A      2.9798 eV  416.08 nm  f=0.0011
<S**2>=0.000
     320 -> 345        0.10068
     324 -> 345        0.63289
     333 -> 346       -0.16566

 Excited State  74:      Singlet-A      2.9990 eV  413.41 nm  f=0.0061
<S**2>=0.000
     324 -> 345        0.13496
     332 -> 348        0.17107
     333 -> 346        0.60243
     333 -> 347       -0.22789
     343 -> 352        0.14724

 Excited State  75:      Singlet-A      3.0094 eV  411.99 nm  f=0.0925
<S**2>=0.000
     332 -> 346        0.61593
     332 -> 347       -0.23135
     333 -> 348        0.21373

 Excited State  76:      Singlet-A      3.0251 eV  409.85 nm  f=0.0001
<S**2>=0.000
     333 -> 346        0.23405
     333 -> 347        0.62229
     334 -> 348       -0.13589

 Excited State  77:      Singlet-A      3.0277 eV  409.49 nm  f=0.2093
<S**2>=0.000
     321 -> 345        0.19386
     323 -> 345        0.55226
     333 -> 348        0.11396
     338 -> 349       -0.12245
     342 -> 351        0.17213
     344 -> 352       -0.24248
```

```
 Excited State  78:      Singlet-A      3.0407 eV  407.75 nm  f=0.0830
<S**2>=0.000
     321 -> 345        0.36332
     323 -> 345       -0.14933
     332 -> 346        0.10845
     332 -> 347        0.32497
     335 -> 348        0.42420

 Excited State  79:      Singlet-A      3.0419 eV  407.59 nm  f=0.0005
<S**2>=0.000
     322 -> 345        0.56838
     331 -> 347        0.11629
     334 -> 348       -0.10273
     343 -> 352        0.35287

 Excited State  80:      Singlet-A      3.0424 eV  407.52 nm  f=0.1014
<S**2>=0.000
     321 -> 345        0.43116
     323 -> 345       -0.31565
     332 -> 346       -0.12471
     332 -> 347       -0.34802
     335 -> 348       -0.18741

 Excited State  81:      Singlet-A      3.0429 eV  407.45 nm  f=0.0005
<S**2>=0.000
     322 -> 345       -0.38656
     330 -> 347        0.12807
     331 -> 346        0.14088
     331 -> 347        0.18575
     343 -> 352        0.48924

 Excited State  82:      Singlet-A      3.0515 eV  406.30 nm  f=0.0010
<S**2>=0.000
     330 -> 346        0.20104
     331 -> 346       -0.41385
     333 -> 347        0.10249
     334 -> 348        0.47795
     335 -> 349       -0.10514

 Excited State  83:      Singlet-A      3.0536 eV  406.02 nm  f=0.0528
<S**2>=0.000
     319 -> 345        0.11634
     321 -> 345       -0.11526
     332 -> 346       -0.18874
     332 -> 347       -0.38798
     334 -> 349       -0.12423
     335 -> 348        0.47607

 Excited State  84:      Singlet-A      3.0539 eV  405.98 nm  f=0.0006
<S**2>=0.000
     322 -> 345        0.12698
     330 -> 346       -0.29305
     331 -> 346        0.43731
     334 -> 348        0.41071

 Excited State  85:      Singlet-A      3.0599 eV  405.19 nm  f=0.0001
<S**2>=0.000
     330 -> 347       -0.38420
```

```
     331 -> 347        0.57581

 Excited State  86:      Singlet-A      3.0725 eV  403.53 nm  f=0.0000
<S**2>=0.000
     342 -> 352        0.69109

 Excited State  87:      Singlet-A      3.0850 eV  401.90 nm  f=0.8455
<S**2>=0.000
     316 -> 345        0.18667
     321 -> 345        0.33996
     323 -> 345        0.23810
     329 -> 346        0.10969
     330 -> 345       -0.10340
     333 -> 348       -0.17641
     336 -> 349       -0.10352
     338 -> 349        0.21951
     342 -> 351       -0.24032
     344 -> 352        0.24728

 Excited State  88:      Singlet-A      3.1047 eV  399.35 nm  f=0.0001
<S**2>=0.000
     328 -> 346        0.18623
     328 -> 347        0.23595
     330 -> 346        0.50970
     330 -> 347       -0.17643
     331 -> 346        0.26202

 Excited State  89:      Singlet-A      3.1180 eV  397.64 nm  f=0.0026
<S**2>=0.000
     320 -> 345        0.54652
     330 -> 347        0.32663
     331 -> 347        0.19046
     332 -> 348        0.13516
     343 -> 352       -0.11296

 Excited State  90:      Singlet-A      3.1242 eV  396.85 nm  f=0.0123
<S**2>=0.000
     327 -> 346       -0.14973
     328 -> 348       -0.13615
     329 -> 346        0.64601
     333 -> 348        0.11523

 Excited State  91:      Singlet-A      3.1298 eV  396.14 nm  f=0.0026
<S**2>=0.000
     320 -> 345       -0.15163
     328 -> 346        0.53784
     328 -> 347       -0.27597
     329 -> 348       -0.13702
     330 -> 347        0.19225
     331 -> 347        0.10573
     344 -> 355        0.14827

 Excited State  92:      Singlet-A      3.1328 eV  395.76 nm  f=0.0173
<S**2>=0.000
     327 -> 347       -0.15418
     328 -> 348        0.10579
     329 -> 347        0.64392
     331 -> 348        0.11476
```

```
 Excited State  93:      Singlet-A      3.1507 eV  393.51 nm  f=0.0040
<S**2>=0.000
     320 -> 345        0.31808
     326 -> 346        0.10610
     328 -> 346        0.30971
     328 -> 347        0.11869
     329 -> 348       -0.14395
     330 -> 346       -0.19704
     330 -> 347       -0.18451
     331 -> 346       -0.11872
     331 -> 347       -0.10310
     332 -> 348       -0.27112
     344 -> 355       -0.15530

 Excited State  94:      Singlet-A      3.1514 eV  393.43 nm  f=0.0016
<S**2>=0.000
     341 -> 351        0.69886

 Excited State  95:      Singlet-A      3.1528 eV  393.25 nm  f=0.0067
<S**2>=0.000
     327 -> 346        0.19854
     340 -> 351        0.66316

 Excited State  96:      Singlet-A      3.1538 eV  393.12 nm  f=0.0019
<S**2>=0.000
     319 -> 345        0.12254
     327 -> 346        0.62653
     327 -> 347        0.11279
     331 -> 348        0.10212
     340 -> 351       -0.18566

 Excited State  97:      Singlet-A      3.1542 eV  393.07 nm  f=0.0006
<S**2>=0.000
     320 -> 345       -0.13170
     328 -> 346        0.12745
     328 -> 347        0.54916
     330 -> 346       -0.13067
     330 -> 347        0.19958
     331 -> 347        0.11604
     332 -> 348        0.10499
     344 -> 354       -0.14283

 Excited State  98:      Singlet-A      3.1597 eV  392.39 nm  f=0.0019
<S**2>=0.000
     319 -> 345        0.16164
     327 -> 346       -0.13774
     327 -> 347        0.62665
     331 -> 348        0.13381
     340 -> 351        0.12965

 Excited State  99:      Singlet-A      3.1694 eV  391.19 nm  f=0.0001
<S**2>=0.000
     319 -> 345       -0.22676
     330 -> 348       -0.24948
     331 -> 348        0.45250
     332 -> 346       -0.10209
     332 -> 349        0.11426
     333 -> 348        0.33990
```

```
 Excited State 100:      Singlet-A      3.1718 eV  390.90 nm  f=0.0250
<S**2>=0.000
     319 -> 345        0.39471
     325 -> 346       -0.12839
     327 -> 347       -0.14848
     330 -> 348       -0.22816
     331 -> 348        0.36054
     333 -> 348       -0.22980

 Excited State 101:      Singlet-A      3.1743 eV  390.58 nm  f=0.0018
<S**2>=0.000
     318 -> 345        0.61472
     326 -> 346       -0.21587
     326 -> 347       -0.14076
     332 -> 348        0.14472

 Excited State 102:      Singlet-A      3.1748 eV  390.52 nm  f=0.0153
<S**2>=0.000
     314 -> 345       -0.10225
     319 -> 345        0.40717
     327 -> 347       -0.10376
     331 -> 348       -0.16570
     332 -> 347        0.13182
     332 -> 349        0.14855
     333 -> 348        0.40082

 Excited State 103:      Singlet-A      3.1831 eV  389.51 nm  f=0.0209
<S**2>=0.000
     318 -> 345       -0.23687
     326 -> 346       -0.23888
     329 -> 348       -0.11717
     330 -> 347       -0.13429
     332 -> 348        0.44957
     333 -> 346       -0.10522
     333 -> 349        0.16553
     344 -> 355       -0.20940

 Excited State 104:      Singlet-A      3.1957 eV  387.97 nm  f=0.0035
<S**2>=0.000
     330 -> 348       -0.22697
     343 -> 354       -0.30447
     344 -> 353        0.58453

 Excited State 105:      Singlet-A      3.1976 eV  387.74 nm  f=0.0000
<S**2>=0.000
     343 -> 353       -0.34249
     344 -> 354        0.59464

 Excited State 106:      Singlet-A      3.2093 eV  386.33 nm  f=0.0048
<S**2>=0.000
     318 -> 345        0.13775
     326 -> 346        0.56867
     326 -> 347        0.12437
     332 -> 348        0.22233
     333 -> 349        0.14833
     335 -> 349        0.10173
     344 -> 355       -0.11439
```

```
 Excited State 107:      Singlet-A      3.2116 eV  386.05 nm  f=0.0787
<S**2>=0.000
     325 -> 346       -0.30788
     329 -> 347       -0.13348
     330 -> 348        0.45523
     331 -> 348        0.21545
     334 -> 349       -0.13763
     343 -> 354       -0.14723
     344 -> 353        0.13135
     344 -> 356        0.19311

 Excited State 108:      Singlet-A      3.2178 eV  385.30 nm  f=0.0021
<S**2>=0.000
     318 -> 345        0.11170
     326 -> 346       -0.13007
     326 -> 347        0.64577

 Excited State 109:      Singlet-A      3.2198 eV  385.07 nm  f=0.0552
<S**2>=0.000
     316 -> 345       -0.10419
     317 -> 345        0.32844
     325 -> 346        0.48384
     325 -> 347        0.14019
     330 -> 348        0.19282
     331 -> 348        0.11064
     344 -> 356        0.15237

 Excited State 110:      Singlet-A      3.2228 eV  384.71 nm  f=0.0152
<S**2>=0.000
     317 -> 345        0.62115
     325 -> 346       -0.25746
     325 -> 347       -0.13546

 Excited State 111:      Singlet-A      3.2303 eV  383.81 nm  f=0.0042
<S**2>=0.000
     325 -> 346       -0.17764
     325 -> 347        0.64269
     326 -> 348        0.10672

 Excited State 112:      Singlet-A      3.2524 eV  381.20 nm  f=0.0022
<S**2>=0.000
     327 -> 348       -0.21889
     329 -> 348        0.15481
     334 -> 348        0.10749
     335 -> 349        0.60493
     343 -> 353        0.17125

 Excited State 113:      Singlet-A      3.2574 eV  380.62 nm  f=0.0045
<S**2>=0.000
     334 -> 349        0.63445
     335 -> 348        0.10984
     343 -> 354       -0.20633

 Excited State 114:      Singlet-A      3.2627 eV  380.00 nm  f=0.0002
<S**2>=0.000
     325 -> 348       -0.13703
     327 -> 348       -0.28484
     329 -> 348        0.36041
     330 -> 347       -0.10130
```

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     333 -> 349        0.13672
     335 -> 349       -0.18305
     342 -> 356        0.11613
     343 -> 352        0.11774
     344 -> 355        0.33838

 Excited State 115:      Singlet-A      3.2653 eV  379.71 nm  f=0.0002
<S**2>=0.000
     327 -> 348        0.36307
     329 -> 348       -0.18776
     334 -> 350       -0.16878
     335 -> 349        0.14182
     342 -> 356        0.14526
     343 -> 352        0.12589
     344 -> 355        0.43059

 Excited State 116:      Singlet-A      3.2659 eV  379.63 nm  f=0.0000
<S**2>=0.000
     315 -> 345        0.70463

 Excited State 117:      Singlet-A      3.2712 eV  379.02 nm  f=0.1143
<S**2>=0.000
     316 -> 345        0.42296
     325 -> 346        0.10215
     326 -> 348       -0.13229
     328 -> 348        0.32765
     332 -> 349       -0.10448
     335 -> 350        0.31184
     343 -> 355       -0.10909

 Excited State 118:      Singlet-A      3.2764 eV  378.42 nm  f=0.0814
<S**2>=0.000
     316 -> 345       -0.40737
     328 -> 348        0.23015
     335 -> 350        0.45861

 Excited State 119:      Singlet-A      3.2799 eV  378.02 nm  f=0.0020
<S**2>=0.000
     327 -> 348        0.34971
     329 -> 348        0.17728
     334 -> 350        0.56326

 Excited State 120:      Singlet-A      3.2898 eV  376.87 nm  f=0.0015
<S**2>=0.000
     324 -> 346       -0.25721
     324 -> 347        0.14689
     330 -> 348       -0.14758
     344 -> 356        0.57131

 Excited State 121:      Singlet-A      3.2960 eV  376.16 nm  f=0.0038
<S**2>=0.000
     316 -> 345        0.12799
     324 -> 346        0.12304
     324 -> 347        0.10829
     328 -> 348       -0.26550
     335 -> 350        0.27867
     342 -> 354       -0.16992
     343 -> 355        0.47439
```

```
 Excited State 122:      Singlet-A      3.3040 eV  375.25 nm  f=0.0001
<S**2>=0.000
     313 -> 345        0.70365

 Excited State 123:      Singlet-A      3.3092 eV  374.67 nm  f=0.0000
<S**2>=0.000
     342 -> 353        0.68770

 Excited State 124:      Singlet-A      3.3095 eV  374.63 nm  f=0.0010
<S**2>=0.000
     341 -> 352        0.11425
     342 -> 354        0.67247
     343 -> 355        0.11725

 Excited State 125:      Singlet-A      3.3143 eV  374.09 nm  f=0.0004
<S**2>=0.000
     341 -> 352        0.67250
     342 -> 354       -0.10621
     342 -> 355        0.10750

 Excited State 126:      Singlet-A      3.3152 eV  373.99 nm  f=0.0000
<S**2>=0.000
     340 -> 352        0.70062

 Excited State 127:      Singlet-A      3.3173 eV  373.75 nm  f=0.0010
<S**2>=0.000
     314 -> 345       -0.32883
     341 -> 352       -0.13847
     342 -> 355        0.59815

 Excited State 128:      Singlet-A      3.3234 eV  373.07 nm  f=0.0303
<S**2>=0.000
     326 -> 348        0.47710
     328 -> 348        0.21696
     329 -> 349       -0.10095
     332 -> 349       -0.20801
     335 -> 350       -0.11406
     343 -> 354        0.21842
     343 -> 355        0.21111
     344 -> 353        0.10515
     344 -> 357       -0.13611

 Excited State 129:      Singlet-A      3.3298 eV  372.35 nm  f=0.0043
<S**2>=0.000
     325 -> 348        0.31374
     327 -> 348        0.21449
     328 -> 349       -0.19597
     329 -> 348        0.31844
     333 -> 349        0.18433
     334 -> 350       -0.24418
     343 -> 353       -0.17711
     343 -> 356       -0.11936
     343 -> 357        0.10453
     344 -> 355       -0.10974

 Excited State 130:      Singlet-A      3.3356 eV  371.71 nm  f=0.0251
<S**2>=0.000
     325 -> 348       -0.28148
     327 -> 348        0.16588
```

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     328 -> 346        0.10399
     328 -> 349       -0.16060
     329 -> 348        0.23126
     333 -> 349       -0.18620
     334 -> 350       -0.19173
     343 -> 353        0.30724
     343 -> 356        0.22617
     344 -> 354        0.16380

 Excited State 131:      Singlet-A      3.3381 eV  371.42 nm  f=0.0639
<S**2>=0.000
     326 -> 348       -0.20179
     328 -> 348        0.28333
     329 -> 349       -0.17231
     332 -> 349        0.21951
     335 -> 350       -0.17416
     343 -> 354       -0.21022
     343 -> 355        0.33161
     344 -> 353       -0.11888
     344 -> 357       -0.19139

 Excited State 132:      Singlet-A      3.3500 eV  370.10 nm  f=0.0084
<S**2>=0.000
     325 -> 348        0.30362
     332 -> 350        0.12778
     333 -> 349        0.19828
     343 -> 356        0.55141

 Excited State 133:      Singlet-A      3.3514 eV  369.94 nm  f=0.0311
<S**2>=0.000
     324 -> 346        0.21788
     324 -> 347       -0.16584
     326 -> 348       -0.28230
     328 -> 350       -0.12931
     332 -> 349        0.14784
     333 -> 350        0.13895
     334 -> 349        0.14941
     343 -> 354        0.39923
     344 -> 353        0.21514

 Excited State 134:      Singlet-A      3.3574 eV  369.28 nm  f=0.0047
<S**2>=0.000
     325 -> 348        0.28942
     329 -> 350        0.15455
     333 -> 349        0.13683
     335 -> 349       -0.14293
     343 -> 353        0.40720
     343 -> 356       -0.27822
     344 -> 354        0.22066

 Excited State 135:      Singlet-A      3.3743 eV  367.44 nm  f=0.0932
<S**2>=0.000
     314 -> 345        0.18800
     324 -> 346        0.45093
     324 -> 347        0.16801
     328 -> 350        0.10047
     331 -> 350       -0.13135
     333 -> 350       -0.31800
     342 -> 355        0.11937
```

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     344 -> 356        0.15919

 Excited State 136:      Singlet-A      3.3825 eV  366.55 nm  f=0.0061
<S**2>=0.000
     324 -> 346       -0.17475
     324 -> 347        0.53488
     326 -> 348       -0.10970
     328 -> 350       -0.12505
     331 -> 350       -0.18077
     343 -> 354        0.12993
     344 -> 356       -0.14372

 Excited State 137:      Singlet-A      3.3862 eV  366.14 nm  f=0.1085
<S**2>=0.000
     314 -> 345       -0.20821
     324 -> 346        0.28675
     324 -> 347        0.18770
     331 -> 350       -0.11274
     333 -> 350        0.46685
     342 -> 355       -0.13675
     343 -> 354       -0.12200

 Excited State 138:      Singlet-A      3.3956 eV  365.13 nm  f=0.0129
<S**2>=0.000
     319 -> 346       -0.10226
     325 -> 348       -0.28871
     326 -> 349        0.11411
     331 -> 349        0.29962
     332 -> 348       -0.16821
     332 -> 350        0.10707
     333 -> 349        0.44295

 Excited State 139:      Singlet-A      3.4022 eV  364.42 nm  f=0.0031
<S**2>=0.000
     325 -> 348        0.12664
     330 -> 349       -0.29114
     331 -> 349        0.56025
     332 -> 350       -0.13650
     333 -> 349       -0.18537

 Excited State 140:      Singlet-A      3.4042 eV  364.21 nm  f=0.0010
<S**2>=0.000
     319 -> 347       -0.13145
     332 -> 350        0.61279
     333 -> 349       -0.16171

 Excited State 141:      Singlet-A      3.4113 eV  363.45 nm  f=0.0023
<S**2>=0.000
     324 -> 347        0.10518
     330 -> 350       -0.34531
     331 -> 350        0.56623
     332 -> 349       -0.12456

 Excited State 142:      Singlet-A      3.4199 eV  362.54 nm  f=0.0002
<S**2>=0.000
     314 -> 345        0.34981
     318 -> 346        0.10112
     326 -> 348        0.17475
     330 -> 350       -0.16084
```

```
     332 -> 349        0.32564
     333 -> 350        0.19908
     342 -> 355        0.20314
     344 -> 357       -0.11515

 Excited State 143:      Singlet-A      3.4209 eV  362.43 nm  f=0.0000
<S**2>=0.000
     314 -> 345       -0.32235
     326 -> 348        0.14290
     330 -> 350       -0.16726
     332 -> 349        0.34882
     333 -> 348       -0.10583
     333 -> 350       -0.22175
     342 -> 355       -0.17728

 Excited State 144:      Singlet-A      3.4289 eV  361.58 nm  f=0.0001
<S**2>=0.000
     321 -> 346       -0.21049
     323 -> 346       -0.39055
     323 -> 347        0.27672
     330 -> 349        0.41571
     331 -> 349        0.12252

 Excited State 145:      Singlet-A      3.4339 eV  361.06 nm  f=0.0008
<S**2>=0.000
     311 -> 346        0.10246
     312 -> 345        0.44326
     321 -> 346        0.11770
     323 -> 346        0.30109
     323 -> 347       -0.15792
     324 -> 348        0.10542
     330 -> 349        0.30561
     331 -> 349        0.14051
     339 -> 351        0.12703

 Excited State 146:      Singlet-A      3.4427 eV  360.14 nm  f=0.0025
<S**2>=0.000
     312 -> 345        0.12382
     321 -> 346        0.53156
     322 -> 348        0.11762
     323 -> 346       -0.35138
     342 -> 356        0.17404

 Excited State 147:      Singlet-A      3.4437 eV  360.04 nm  f=0.0204
<S**2>=0.000
     311 -> 345        0.15818
     322 -> 346        0.63177
     323 -> 348       -0.10058
     330 -> 350       -0.10902
     344 -> 357       -0.15165

 Excited State 148:      Singlet-A      3.4472 eV  359.66 nm  f=0.0000
<S**2>=0.000
     312 -> 345        0.23938
     321 -> 347       -0.24151
     323 -> 346        0.12247
     323 -> 347        0.53713
     330 -> 349       -0.18046
     339 -> 351       -0.10504
```

```
 Excited State 149:      Singlet-A      3.4481 eV  359.57 nm  f=0.0351
<S**2>=0.000
     311 -> 345        0.63582
     312 -> 346        0.16720
     316 -> 345       -0.10036
     322 -> 346       -0.15793

 Excited State 150:      Singlet-A      3.4512 eV  359.25 nm  f=0.0080
<S**2>=0.000
     322 -> 346        0.10191
     322 -> 347        0.66800
     344 -> 357        0.12450

 Excited State 151:      Singlet-A      3.4513 eV  359.24 nm  f=0.0001
<S**2>=0.000
     312 -> 345        0.39296
     321 -> 346       -0.21553
     321 -> 347        0.14308
     323 -> 346       -0.22795
     323 -> 347       -0.17482
     330 -> 349       -0.21693
     331 -> 349       -0.11431
     339 -> 351       -0.20562
     342 -> 356       -0.18192

 Excited State 152:      Singlet-A      3.4557 eV  358.78 nm  f=0.0001
<S**2>=0.000
     308 -> 345       -0.15224
     310 -> 345       -0.30168
     319 -> 346        0.14346
     321 -> 346       -0.27158
     323 -> 347       -0.14099
     342 -> 356        0.45133

 Excited State 153:      Singlet-A      3.4574 eV  358.60 nm  f=0.0500
<S**2>=0.000
     322 -> 346       -0.15297
     322 -> 347        0.17019
     329 -> 349        0.35509
     330 -> 350       -0.32586
     331 -> 350       -0.13538
     332 -> 349       -0.16061
     344 -> 357       -0.32993

 Excited State 154:      Singlet-A      3.4706 eV  357.24 nm  f=0.0020
<S**2>=0.000
     321 -> 347        0.60666
     322 -> 348       -0.10638
     323 -> 346        0.15863
     323 -> 347        0.20708

 Excited State 155:      Singlet-A      3.4783 eV  356.45 nm  f=0.0002
<S**2>=0.000
     324 -> 348        0.51795
     329 -> 350        0.43550

 Excited State 156:      Singlet-A      3.4930 eV  354.95 nm  f=0.0127
<S**2>=0.000
```

```
     320 -> 346        0.15254
     320 -> 347        0.25920
     324 -> 347        0.15471
     327 -> 349       -0.31126
     329 -> 349        0.32696
     330 -> 350        0.28733
     331 -> 350        0.22653

 Excited State 157:      Singlet-A      3.4957 eV  354.68 nm  f=0.0061
<S**2>=0.000
     310 -> 345       -0.12514
     327 -> 350        0.10939
     328 -> 349        0.51789
     343 -> 357        0.38310

 Excited State 158:      Singlet-A      3.4975 eV  354.50 nm  f=0.0259
<S**2>=0.000
     318 -> 346       -0.11054
     320 -> 346        0.12005
     320 -> 347        0.20704
     327 -> 349        0.54592
     330 -> 350        0.17556
     344 -> 357       -0.23623

 Excited State 159:      Singlet-A      3.4995 eV  354.29 nm  f=0.0004
<S**2>=0.000
     324 -> 348        0.32256
     327 -> 350        0.46088
     329 -> 350       -0.34925
     343 -> 357       -0.11402

 Excited State 160:      Singlet-A      3.5033 eV  353.91 nm  f=0.0623
<S**2>=0.000
     320 -> 346       -0.29292
     320 -> 347        0.15422
     328 -> 350        0.58097
     343 -> 354        0.11912

 Excited State 161:      Singlet-A      3.5082 eV  353.41 nm  f=0.0005
<S**2>=0.000
     309 -> 345        0.70528

 Excited State 162:      Singlet-A      3.5103 eV  353.20 nm  f=0.0000
<S**2>=0.000
     308 -> 345        0.62156
     310 -> 345       -0.33550

 Excited State 163:      Singlet-A      3.5248 eV  351.74 nm  f=0.0005
<S**2>=0.000
     320 -> 348       -0.10283
     324 -> 348       -0.22369
     327 -> 350        0.49070
     329 -> 350        0.31089
     339 -> 351        0.20783
     343 -> 353       -0.10248

 Excited State 164:      Singlet-A      3.5370 eV  350.54 nm  f=0.0130
<S**2>=0.000
     307 -> 345        0.37405
```

```
     320 -> 346        0.42505
     320 -> 347       -0.17755
     323 -> 348        0.11869
     326 -> 350        0.11332
     328 -> 350        0.24255

 Excited State 165:      Singlet-A      3.5397 eV  350.27 nm  f=0.0003
<S**2>=0.000
     308 -> 345        0.13266
     310 -> 345        0.22039
     319 -> 346        0.28799
     319 -> 347       -0.10575
     325 -> 350       -0.10182
     326 -> 349        0.49718
     328 -> 349        0.10898
     339 -> 351       -0.18762

 Excited State 166:      Singlet-A      3.5400 eV  350.23 nm  f=0.0025
<S**2>=0.000
     307 -> 345        0.59420
     320 -> 346       -0.28054
     328 -> 350       -0.14451

 Excited State 167:      Singlet-A      3.5452 eV  349.72 nm  f=0.0075
<S**2>=0.000
     318 -> 346        0.24289
     320 -> 346        0.13094
     320 -> 347        0.30662
     325 -> 349        0.22432
     326 -> 350       -0.25271
     327 -> 349        0.15314
     329 -> 349        0.16965
     330 -> 350       -0.11084
     339 -> 352        0.18343
     343 -> 355        0.10829
     344 -> 357        0.25354

 Excited State 168:      Singlet-A      3.5525 eV  349.00 nm  f=0.0018
<S**2>=0.000
     310 -> 345        0.11149
     316 -> 346       -0.19904
     319 -> 346        0.13237
     319 -> 347       -0.12677
     327 -> 350       -0.11363
     329 -> 350       -0.13756
     330 -> 349       -0.18471
     331 -> 349       -0.11971
     339 -> 351        0.50782
     342 -> 357       -0.14481

 Excited State 169:      Singlet-A      3.5597 eV  348.30 nm  f=0.0329
<S**2>=0.000
     318 -> 346        0.11969
     318 -> 347       -0.15092
     320 -> 347        0.30463
     321 -> 348       -0.22139
     323 -> 348        0.12127
     325 -> 349        0.15421
     326 -> 350        0.41016
```

```
     327 -> 349       -0.13829
     329 -> 349       -0.19688

 Excited State 170:      Singlet-A      3.5616 eV  348.11 nm  f=0.0061
<S**2>=0.000
     310 -> 345        0.14381
     318 -> 348       -0.18521
     319 -> 346        0.25877
     319 -> 347       -0.10801
     326 -> 349       -0.31251
     342 -> 357        0.42902
     343 -> 357        0.14917

 Excited State 171:      Singlet-A      3.5616 eV  348.11 nm  f=0.0005
<S**2>=0.000
     320 -> 347        0.11464
     321 -> 348        0.22190
     323 -> 348        0.54487
     326 -> 350       -0.23138
     329 -> 349       -0.14413

 Excited State 172:      Singlet-A      3.5633 eV  347.94 nm  f=0.0026
<S**2>=0.000
     310 -> 345       -0.10822
     316 -> 347        0.11381
     318 -> 348        0.13241
     319 -> 346       -0.17142
     326 -> 349        0.27101
     339 -> 351        0.17168
     342 -> 357        0.52422

 Excited State 173:      Singlet-A      3.5698 eV  347.32 nm  f=0.0014
<S**2>=0.000
     320 -> 347       -0.11219
     325 -> 349        0.61025
     326 -> 350       -0.13243
     330 -> 350        0.10546
     339 -> 352       -0.15389
     344 -> 357       -0.11498

 Excited State 174:      Singlet-A      3.5720 eV  347.10 nm  f=0.0173
<S**2>=0.000
     320 -> 346       -0.14410
     321 -> 348        0.42955
     323 -> 348        0.11183
     325 -> 349        0.12041
     326 -> 350        0.37982
     327 -> 349        0.10766
     329 -> 349        0.18039
     344 -> 357        0.12630

 Excited State 175:      Singlet-A      3.5731 eV  346.99 nm  f=0.0070
<S**2>=0.000
     322 -> 348        0.22988
     325 -> 350        0.43616
     326 -> 349        0.17237
     328 -> 349       -0.20076
     343 -> 357        0.32734
```

```
 Excited State 176:      Singlet-A      3.5748 eV  346.83 nm  f=0.0004
<S**2>=0.000
     340 -> 354        0.36835
     341 -> 353        0.59684

 Excited State 177:      Singlet-A      3.5750 eV  346.81 nm  f=0.0000
<S**2>=0.000
     340 -> 353        0.49108
     341 -> 354        0.50304

 Excited State 178:      Singlet-A      3.5789 eV  346.43 nm  f=0.0110
<S**2>=0.000
     340 -> 353        0.49535
     341 -> 354       -0.47659

 Excited State 179:      Singlet-A      3.5791 eV  346.41 nm  f=0.0012
<S**2>=0.000
     340 -> 354        0.59287
     341 -> 353       -0.35520

 Excited State 180:      Singlet-A      3.5810 eV  346.23 nm  f=0.0003
<S**2>=0.000
     319 -> 347       -0.14968
     322 -> 348       -0.29151
     325 -> 350        0.49422
     328 -> 349        0.15224
     343 -> 357       -0.19267

 Excited State 181:      Singlet-A      3.5833 eV  346.00 nm  f=0.0013
<S**2>=0.000
     318 -> 346        0.44181
     318 -> 347       -0.19746
     319 -> 348       -0.38650
     320 -> 347       -0.17308
     339 -> 352       -0.15662
     344 -> 357       -0.11258

 Excited State 182:      Singlet-A      3.5834 eV  346.00 nm  f=0.0002
<S**2>=0.000
     306 -> 345        0.69885

 Excited State 183:      Singlet-A      3.5858 eV  345.77 nm  f=0.0003
<S**2>=0.000
     305 -> 345        0.70455

 Excited State 184:      Singlet-A      3.5900 eV  345.36 nm  f=0.0017
<S**2>=0.000
     341 -> 355        0.69822

 Excited State 185:      Singlet-A      3.5911 eV  345.25 nm  f=0.0002
<S**2>=0.000
     340 -> 355        0.70240

 Excited State 186:      Singlet-A      3.5951 eV  344.87 nm  f=0.0021
<S**2>=0.000
     308 -> 345       -0.15008
     310 -> 345       -0.26761
     314 -> 346       -0.14971
     318 -> 348       -0.15656
```

```
     319 -> 346        0.20769
     322 -> 348        0.38456
     338 -> 351        0.23902
     342 -> 356       -0.17182

 Excited State 187:      Singlet-A      3.6069 eV  343.74 nm  f=0.0000
<S**2>=0.000
     317 -> 346        0.69313

 Excited State 188:      Singlet-A      3.6105 eV  343.40 nm  f=0.0012
<S**2>=0.000
     320 -> 347        0.22032
     321 -> 348        0.40263
     322 -> 346       -0.12296
     322 -> 349        0.14451
     323 -> 348       -0.34462
     327 -> 349       -0.10970
     328 -> 348       -0.10590
     329 -> 349       -0.16795
     344 -> 357       -0.10459

 Excited State 189:      Singlet-A      3.6123 eV  343.23 nm  f=0.0048
<S**2>=0.000
     310 -> 345       -0.10160
     317 -> 346       -0.10129
     317 -> 347        0.60752
     322 -> 348       -0.15530
     328 -> 349       -0.11319
     343 -> 357        0.14588

 Excited State 190:      Singlet-A      3.6166 eV  342.82 nm  f=0.0197
<S**2>=0.000
     310 -> 345        0.15864
     314 -> 346        0.12777
     317 -> 347        0.33908
     318 -> 348        0.11924
     322 -> 348        0.33282
     328 -> 349        0.18512
     342 -> 356        0.11963
     343 -> 357       -0.24134

 Excited State 191:      Singlet-A      3.6253 eV  342.00 nm  f=0.0022
<S**2>=0.000
     341 -> 356        0.70343

 Excited State 192:      Singlet-A      3.6265 eV  341.88 nm  f=0.0033
<S**2>=0.000
     340 -> 356        0.69669

 Excited State 193:      Singlet-A      3.6325 eV  341.32 nm  f=0.0000
<S**2>=0.000
     316 -> 346        0.12447
     318 -> 350       -0.15195
     319 -> 346       -0.16219
     319 -> 347       -0.38048
     320 -> 348        0.47855
     325 -> 350       -0.12176
```

```
 Excited State 194:      Singlet-A      3.6427 eV  340.37 nm  f=0.0000
<S**2>=0.000
     316 -> 346        0.41549
     316 -> 347       -0.18490
     318 -> 350        0.13627
     319 -> 346        0.15999
     319 -> 347        0.31966
     320 -> 348        0.25062
     339 -> 351        0.13976

 Excited State 195:      Singlet-A      3.6528 eV  339.43 nm  f=0.0142
<S**2>=0.000
     315 -> 346        0.65339
     315 -> 347        0.17679
     318 -> 347        0.15274

 Excited State 196:      Singlet-A      3.6558 eV  339.14 nm  f=0.1138
<S**2>=0.000
     315 -> 346       -0.24076
     315 -> 347        0.15750
     316 -> 348        0.12121
     318 -> 346        0.22425
     318 -> 347        0.48613
     319 -> 350        0.24254
     326 -> 350        0.11132

 Excited State 197:      Singlet-A      3.6594 eV  338.81 nm  f=0.0134
<S**2>=0.000
     315 -> 346       -0.11570
     315 -> 347        0.66567
     318 -> 347       -0.15435

 Excited State 198:      Singlet-A      3.6662 eV  338.19 nm  f=0.0020
<S**2>=0.000
     311 -> 347       -0.12099
     314 -> 346       -0.11376
     316 -> 346        0.25784
     316 -> 347        0.52609
     318 -> 348       -0.17527
     324 -> 350        0.16852
     338 -> 351       -0.15298

 Excited State 199:      Singlet-A      3.6916 eV  335.86 nm  f=0.0005
<S**2>=0.000
     313 -> 346        0.70202

 Excited State 200:      Singlet-A      3.6997 eV  335.12 nm  f=0.0017
<S**2>=0.000
     313 -> 347        0.70275
```

4b – CH_2Cl_2 BP86/6-31+G(d)

```
Excited State   1:      Singlet-A      1.3192 eV  939.81 nm  f=0.0000
<S**2>=0.000
     342 -> 346        0.11582
     343 -> 347       -0.14573
     344 -> 345        0.67248
 This state for optimization and/or second-order correction.
```

```
 Total Energy, E(TD-HF/TD-DFT) =  -4240.58811143
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      1.3287 eV  933.12 nm  f=0.4140
<S**2>=0.000
     343 -> 345        0.68236
     344 -> 347       -0.15959

 Excited State   3:      Singlet-A      1.5745 eV  787.46 nm  f=0.1453
<S**2>=0.000
     340 -> 345        0.25226
     342 -> 345        0.47737
     343 -> 348        0.13656
     344 -> 346        0.37220
     344 -> 347       -0.18263
     344 -> 349        0.10356

 Excited State   4:      Singlet-A      1.5943 eV  777.70 nm  f=0.0000
<S**2>=0.000
     341 -> 345        0.70536

 Excited State   5:      Singlet-A      1.5982 eV  775.78 nm  f=0.0198
<S**2>=0.000
     340 -> 345        0.65639
     342 -> 345       -0.14225
     344 -> 346       -0.17600

 Excited State   6:      Singlet-A      1.6753 eV  740.06 nm  f=0.0000
<S**2>=0.000
     343 -> 346        0.51210
     343 -> 347       -0.25115
     344 -> 348        0.41113

 Excited State   7:      Singlet-A      1.7148 eV  723.00 nm  f=0.1508
<S**2>=0.000
     342 -> 345        0.41849
     342 -> 350       -0.16681
     343 -> 348       -0.29189
     344 -> 346       -0.40062
     344 -> 347        0.14214
     344 -> 349        0.15279

 Excited State   8:      Singlet-A      1.7299 eV  716.72 nm  f=0.9014
<S**2>=0.000
     342 -> 348       -0.12382
     343 -> 345        0.15295
     343 -> 350        0.22758
     344 -> 346        0.25189
     344 -> 347        0.58438

 Excited State   9:      Singlet-A      1.7464 eV  709.95 nm  f=0.0000
<S**2>=0.000
     342 -> 346        0.37151
     342 -> 347        0.58510
     344 -> 348        0.10721

 Excited State  10:      Singlet-A      1.7633 eV  703.15 nm  f=0.0000
<S**2>=0.000
```

```
     339 -> 345       -0.18941
     342 -> 346        0.39695
     342 -> 347       -0.28847
     343 -> 346        0.17482
     343 -> 347        0.36709
     344 -> 350        0.22414

 Excited State  11:      Singlet-A      1.8509 eV  669.86 nm  f=0.0000
<S**2>=0.000
     339 -> 345        0.18679
     342 -> 346       -0.34849
     342 -> 347        0.19571
     342 -> 349        0.11812
     343 -> 346        0.18416
     343 -> 347        0.36474
     344 -> 345        0.14836
     344 -> 350        0.31598

 Excited State  12:      Singlet-A      1.8596 eV  666.71 nm  f=0.2717
<S**2>=0.000
     342 -> 348        0.69406

 Excited State  13:      Singlet-A      1.8930 eV  654.97 nm  f=0.0000
<S**2>=0.000
     343 -> 346       -0.28796
     343 -> 347        0.14753
     343 -> 349       -0.42117
     344 -> 348        0.44625

 Excited State  14:      Singlet-A      1.9186 eV  646.23 nm  f=0.0023
<S**2>=0.000
     342 -> 345       -0.13551
     342 -> 350        0.24847
     343 -> 348       -0.40165
     344 -> 346        0.18280
     344 -> 349        0.46033

 Excited State  15:      Singlet-A      1.9871 eV  623.94 nm  f=0.0018
<S**2>=0.000
     340 -> 346        0.26272
     341 -> 346        0.64248

 Excited State  16:      Singlet-A      1.9874 eV  623.85 nm  f=0.0007
<S**2>=0.000
     339 -> 345        0.19911
     340 -> 346        0.57901
     340 -> 347       -0.11141
     341 -> 346       -0.28660
     342 -> 349       -0.12963

 Excited State  17:      Singlet-A      1.9933 eV  622.01 nm  f=0.0002
<S**2>=0.000
     339 -> 345        0.35277
     340 -> 346       -0.27585
     340 -> 347       -0.28704
     341 -> 347        0.32316
     342 -> 349       -0.28436
     344 -> 350        0.11914
```

```
 Excited State  18:      Singlet-A      1.9941 eV  621.75 nm  f=0.0009
<S**2>=0.000
     339 -> 345       -0.15873
     340 -> 346        0.12046
     340 -> 347        0.22162
     341 -> 347        0.62031
     342 -> 349        0.13078

 Excited State  19:      Singlet-A      1.9965 eV  621.02 nm  f=0.0000
<S**2>=0.000
     339 -> 345        0.26622
     340 -> 347        0.59305
     342 -> 349       -0.23013

 Excited State  20:      Singlet-A      2.1079 eV  588.18 nm  f=0.0004
<S**2>=0.000
     341 -> 348        0.69523

 Excited State  21:      Singlet-A      2.1097 eV  587.69 nm  f=0.0005
<S**2>=0.000
     340 -> 348        0.70407

 Excited State  22:      Singlet-A      2.1363 eV  580.37 nm  f=0.0000
<S**2>=0.000
     338 -> 345        0.23186
     341 -> 348       -0.11471
     342 -> 349        0.32780
     343 -> 346       -0.13327
     343 -> 347       -0.25481
     344 -> 345       -0.12570
     344 -> 350        0.44188

 Excited State  23:      Singlet-A      2.1429 eV  578.57 nm  f=0.0001
<S**2>=0.000
     338 -> 345        0.64312
     342 -> 349       -0.12460
     343 -> 349       -0.12575
     344 -> 350       -0.15364

 Excited State  24:      Singlet-A      2.1612 eV  573.69 nm  f=0.3834
<S**2>=0.000
     339 -> 346        0.30869
     339 -> 347       -0.10140
     343 -> 348        0.38134
     343 -> 350        0.10520
     344 -> 346       -0.16084
     344 -> 349        0.42788

 Excited State  25:      Singlet-A      2.1767 eV  569.59 nm  f=0.5971
<S**2>=0.000
     339 -> 347        0.27337
     343 -> 350        0.59271
     344 -> 347       -0.17231

 Excited State  26:      Singlet-A      2.1937 eV  565.17 nm  f=0.0249
<S**2>=0.000
     337 -> 345        0.14400
     339 -> 346       -0.15711
     339 -> 349       -0.12210
```

```
     342 -> 345        0.16033
     342 -> 350        0.58173
     343 -> 348        0.18613
     344 -> 346       -0.14975

 Excited State  27:      Singlet-A      2.1973 eV  564.26 nm  f=0.0000
<S**2>=0.000
     336 -> 345       -0.10430
     338 -> 345        0.11034
     339 -> 348       -0.23838
     343 -> 346       -0.19233
     343 -> 347        0.11569
     343 -> 349        0.51282
     344 -> 348        0.29637

 Excited State  28:      Singlet-A      2.2142 eV  559.95 nm  f=0.0202
<S**2>=0.000
     337 -> 345        0.68720
     342 -> 350       -0.11392

 Excited State  29:      Singlet-A      2.2246 eV  557.32 nm  f=0.0001
<S**2>=0.000
     336 -> 345        0.69074
     338 -> 345        0.10584

 Excited State  30:      Singlet-A      2.3323 eV  531.59 nm  f=0.0045
<S**2>=0.000
     340 -> 349       -0.12248
     341 -> 349        0.69556

 Excited State  31:      Singlet-A      2.3327 eV  531.51 nm  f=0.0001
<S**2>=0.000
     340 -> 349        0.69341
     341 -> 349        0.12341

 Excited State  32:      Singlet-A      2.3445 eV  528.82 nm  f=0.0001
<S**2>=0.000
     341 -> 350        0.70484

 Excited State  33:      Singlet-A      2.3464 eV  528.40 nm  f=0.0003
<S**2>=0.000
     340 -> 350        0.70465

 Excited State  34:      Singlet-A      2.4327 eV  509.65 nm  f=0.1655
<S**2>=0.000
     330 -> 345        0.11693
     338 -> 346        0.15504
     339 -> 346        0.29472
     339 -> 347        0.52698
     343 -> 350       -0.21371

 Excited State  35:      Singlet-A      2.4943 eV  497.07 nm  f=0.1758
<S**2>=0.000
     333 -> 345       -0.10693
     335 -> 345        0.57422
     338 -> 347       -0.11337
     339 -> 346       -0.24298
     339 -> 347        0.18148
     339 -> 349        0.10533
```

```
     344 -> 349        0.10671

 Excited State  36:      Singlet-A      2.5009 eV  495.76 nm  f=0.0001
<S**2>=0.000
     334 -> 345        0.70047

 Excited State  37:      Singlet-A      2.5055 eV  494.85 nm  f=0.4243
<S**2>=0.000
     333 -> 345        0.16585
     335 -> 345        0.38112
     339 -> 346        0.40014
     339 -> 347       -0.19495
     339 -> 349       -0.17910
     342 -> 350        0.12952
     343 -> 348       -0.12110
     344 -> 349       -0.16748

 Excited State  38:      Singlet-A      2.5167 eV  492.64 nm  f=0.0000
<S**2>=0.000
     332 -> 345       -0.11333
     339 -> 348        0.64227
     343 -> 349        0.14269
     344 -> 348        0.12514

 Excited State  39:      Singlet-A      2.5471 eV  486.76 nm  f=0.3191
<S**2>=0.000
     330 -> 345       -0.17275
     336 -> 346       -0.12270
     338 -> 346        0.60870
     338 -> 347       -0.19405
     339 -> 347       -0.10052

 Excited State  40:      Singlet-A      2.5572 eV  484.84 nm  f=0.0000
<S**2>=0.000
     337 -> 346        0.10132
     338 -> 348        0.10660
     339 -> 345        0.32839
     339 -> 350       -0.28352
     342 -> 346        0.16608
     342 -> 349        0.34898
     343 -> 347        0.12382
     344 -> 350       -0.25322

 Excited State  41:      Singlet-A      2.5805 eV  480.47 nm  f=0.1326
<S**2>=0.000
     336 -> 346       -0.16882
     336 -> 347       -0.25717
     338 -> 346        0.18417
     338 -> 347        0.58478

 Excited State  42:      Singlet-A      2.5990 eV  477.05 nm  f=0.0958
<S**2>=0.000
     333 -> 345        0.66425
     339 -> 349        0.10241

 Excited State  43:      Singlet-A      2.6050 eV  475.94 nm  f=0.0000
<S**2>=0.000
     332 -> 345       -0.21482
     337 -> 346        0.65981
```

```
 Excited State  44:      Singlet-A      2.6122 eV  474.64 nm  f=0.0003
<S**2>=0.000
     332 -> 345        0.49710
     337 -> 346        0.13527
     337 -> 347       -0.46704

 Excited State  45:      Singlet-A      2.6144 eV  474.24 nm  f=0.0000
<S**2>=0.000
     332 -> 345        0.42911
     337 -> 346        0.15977
     337 -> 347        0.52356

 Excited State  46:      Singlet-A      2.6172 eV  473.72 nm  f=0.0660
<S**2>=0.000
     336 -> 346        0.61707
     336 -> 347       -0.29496

 Excited State  47:      Singlet-A      2.6346 eV  470.60 nm  f=0.0848
<S**2>=0.000
     336 -> 346        0.24118
     336 -> 347        0.58349
     338 -> 346        0.12354
     338 -> 347        0.26739

 Excited State  48:      Singlet-A      2.6502 eV  467.82 nm  f=0.0000
<S**2>=0.000
     338 -> 348        0.67880
     339 -> 350        0.10110

 Excited State  49:      Singlet-A      2.6667 eV  464.94 nm  f=0.0000
<S**2>=0.000
     331 -> 345        0.70611

 Excited State  50:      Singlet-A      2.7151 eV  456.65 nm  f=0.0765
<S**2>=0.000
     329 -> 345        0.11445
     330 -> 345        0.61730
     338 -> 349       -0.19475
     342 -> 351       -0.14315

 Excited State  51:      Singlet-A      2.7266 eV  454.71 nm  f=0.0105
<S**2>=0.000
     329 -> 345       -0.34859
     330 -> 345        0.10434
     337 -> 348        0.59978

 Excited State  52:      Singlet-A      2.7310 eV  453.98 nm  f=0.0638
<S**2>=0.000
     327 -> 345        0.10353
     329 -> 345        0.58143
     337 -> 348        0.36024

 Excited State  53:      Singlet-A      2.7331 eV  453.64 nm  f=0.0007
<S**2>=0.000
     328 -> 345        0.49880
     336 -> 348        0.48748
```

```
 Excited State  54:      Singlet-A      2.7391 eV  452.64 nm  f=0.0000
<S**2>=0.000
     328 -> 345       -0.47320
     336 -> 348        0.50345
     344 -> 351       -0.10786

 Excited State  55:      Singlet-A      2.7627 eV  448.78 nm  f=0.0442
<S**2>=0.000
     327 -> 345        0.69087

 Excited State  56:      Singlet-A      2.8040 eV  442.17 nm  f=0.0000
<S**2>=0.000
     326 -> 345        0.56987
     339 -> 350        0.26693
     344 -> 351       -0.26839

 Excited State  57:      Singlet-A      2.8132 eV  440.73 nm  f=0.0001
<S**2>=0.000
     324 -> 345        0.14747
     339 -> 345        0.11285
     339 -> 350        0.43448
     342 -> 349        0.12620
     344 -> 351        0.44437

 Excited State  58:      Singlet-A      2.8152 eV  440.42 nm  f=0.0309
<S**2>=0.000
     325 -> 345        0.64728
     339 -> 349       -0.24851

 Excited State  59:      Singlet-A      2.8165 eV  440.20 nm  f=0.0001
<S**2>=0.000
     324 -> 345       -0.11267
     326 -> 345        0.40587
     339 -> 350       -0.30043
     344 -> 351        0.40829

 Excited State  60:      Singlet-A      2.8476 eV  435.40 nm  f=0.0641
<S**2>=0.000
     314 -> 345       -0.10705
     325 -> 345        0.26802
     339 -> 346        0.12908
     339 -> 349        0.56965
     342 -> 350        0.11253

 Excited State  61:      Singlet-A      2.8685 eV  432.23 nm  f=0.0000
<S**2>=0.000
     338 -> 350        0.68717
     344 -> 351       -0.11257

 Excited State  62:      Singlet-A      2.8834 eV  429.99 nm  f=0.0759
<S**2>=0.000
     343 -> 351        0.67096

 Excited State  63:      Singlet-A      2.8921 eV  428.70 nm  f=0.0038
<S**2>=0.000
     334 -> 346       -0.13827
     336 -> 349       -0.10631
     338 -> 349        0.48818
     342 -> 351       -0.45152
```

```
 Excited State  64:      Singlet-A      2.8960 eV  428.12 nm  f=0.0000
<S**2>=0.000
     334 -> 348       -0.16023
     335 -> 346        0.63295
     335 -> 347       -0.25674

 Excited State  65:      Singlet-A      2.8995 eV  427.60 nm  f=0.0077
<S**2>=0.000
     334 -> 346        0.61256
     334 -> 347       -0.23912
     335 -> 348       -0.16576
     342 -> 351       -0.14954

 Excited State  66:      Singlet-A      2.9283 eV  423.40 nm  f=0.0252
<S**2>=0.000
     334 -> 346       -0.14225
     334 -> 347       -0.41066
     335 -> 346        0.17065
     335 -> 347        0.42038
     336 -> 349       -0.10218
     338 -> 349        0.12635
     342 -> 351        0.13101
     344 -> 352       -0.17566

 Excited State  67:      Singlet-A      2.9287 eV  423.35 nm  f=0.0207
<S**2>=0.000
     334 -> 346        0.12537
     334 -> 347        0.36472
     335 -> 346        0.19192
     335 -> 347        0.47127
     338 -> 349       -0.11425
     342 -> 351       -0.12069
     344 -> 352        0.16061

 Excited State  68:      Singlet-A      2.9367 eV  422.19 nm  f=0.0614
<S**2>=0.000
     334 -> 346       -0.17149
     334 -> 347       -0.31436
     336 -> 349        0.24397
     338 -> 349       -0.20766
     342 -> 351       -0.28621
     344 -> 352        0.38976

 Excited State  69:      Singlet-A      2.9508 eV  420.17 nm  f=0.0001
<S**2>=0.000
     337 -> 349        0.70232

 Excited State  70:      Singlet-A      2.9632 eV  418.41 nm  f=0.0104
<S**2>=0.000
     334 -> 347       -0.10985
     336 -> 349       -0.10638
     337 -> 350        0.67573
     344 -> 352        0.11087

 Excited State  71:      Singlet-A      2.9646 eV  418.21 nm  f=0.0002
<S**2>=0.000
     336 -> 349        0.60754
     337 -> 350        0.14563
```

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     338 -> 349        0.11557
     344 -> 352       -0.29053

 Excited State  72:      Singlet-A      2.9720 eV  417.17 nm  f=0.0001
<S**2>=0.000
     336 -> 350        0.69600

 Excited State  73:      Singlet-A      2.9849 eV  415.38 nm  f=0.0000
<S**2>=0.000
     324 -> 345        0.61028
     333 -> 346       -0.24514

 Excited State  74:      Singlet-A      2.9980 eV  413.55 nm  f=0.0000
<S**2>=0.000
     324 -> 345        0.21664
     332 -> 348        0.16055
     333 -> 346        0.57473
     333 -> 347       -0.22422
     343 -> 352        0.15289

 Excited State  75:      Singlet-A      3.0080 eV  412.19 nm  f=0.1100
<S**2>=0.000
     323 -> 345       -0.11338
     332 -> 346        0.61156
     332 -> 347       -0.22894
     333 -> 348        0.20911

 Excited State  76:      Singlet-A      3.0213 eV  410.36 nm  f=0.1685
<S**2>=0.000
     323 -> 345        0.58314
     333 -> 348        0.11897
     338 -> 349       -0.11088
     342 -> 351       -0.16417
     344 -> 352       -0.24683

 Excited State  77:      Singlet-A      3.0233 eV  410.10 nm  f=0.0000
<S**2>=0.000
     333 -> 346        0.23553
     333 -> 347        0.62573
     334 -> 348        0.12051

 Excited State  78:      Singlet-A      3.0405 eV  407.78 nm  f=0.0001
<S**2>=0.000
     322 -> 345        0.66994
     343 -> 352        0.17224

 Excited State  79:      Singlet-A      3.0408 eV  407.74 nm  f=0.0813
<S**2>=0.000
     319 -> 345        0.10425
     321 -> 345        0.32991
     332 -> 346        0.15062
     332 -> 347        0.42465
     335 -> 348       -0.38395

 Excited State  80:      Singlet-A      3.0427 eV  407.48 nm  f=0.0716
<S**2>=0.000
     321 -> 345        0.57458
     323 -> 345       -0.16078
     332 -> 346       -0.11833
```

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     332 -> 347       -0.30730

 Excited State  81:      Singlet-A      3.0428 eV  407.47 nm  f=0.0002
<S**2>=0.000
     322 -> 345       -0.18095
     330 -> 346       -0.14183
     330 -> 347       -0.24855
     343 -> 352        0.58472
     344 -> 355       -0.11832

 Excited State  82:      Singlet-A      3.0536 eV  406.03 nm  f=0.0090
<S**2>=0.000
     331 -> 346        0.66495
     332 -> 347        0.11579
     335 -> 348        0.16864

 Excited State  83:      Singlet-A      3.0545 eV  405.91 nm  f=0.0144
<S**2>=0.000
     331 -> 346        0.14407
     332 -> 347       -0.19028
     334 -> 348        0.49019
     335 -> 348       -0.32283
     335 -> 349        0.11332

 Excited State  84:      Singlet-A      3.0546 eV  405.89 nm  f=0.0199
<S**2>=0.000
     331 -> 346       -0.16337
     332 -> 346        0.11369
     332 -> 347        0.22521
     334 -> 348        0.41197
     335 -> 348        0.38645

 Excited State  85:      Singlet-A      3.0603 eV  405.13 nm  f=0.0135
<S**2>=0.000
     331 -> 347        0.68940

 Excited State  86:      Singlet-A      3.0727 eV  403.50 nm  f=0.0000
<S**2>=0.000
     342 -> 352        0.68924

 Excited State  87:      Singlet-A      3.0825 eV  402.22 nm  f=0.9228
<S**2>=0.000
     316 -> 345       -0.19026
     321 -> 345        0.17822
     323 -> 345        0.32501
     330 -> 345        0.12939
     333 -> 348       -0.18198
     336 -> 349        0.10697
     338 -> 349        0.23171
     342 -> 351        0.25477
     344 -> 352        0.26399

 Excited State  88:      Singlet-A      3.1021 eV  399.68 nm  f=0.0000
<S**2>=0.000
     329 -> 346        0.22714
     329 -> 347        0.23684
     330 -> 346        0.55999
     330 -> 347       -0.18652
```

```
 Excited State  89:      Singlet-A      3.1190 eV  397.51 nm  f=0.0000
<S**2>=0.000
     320 -> 345        0.53668
     330 -> 346        0.11058
     330 -> 347        0.38348
     332 -> 348       -0.14492
     343 -> 352        0.11918

 Excited State  90:      Singlet-A      3.1246 eV  396.80 nm  f=0.0000
<S**2>=0.000
     320 -> 345       -0.10687
     328 -> 348       -0.13486
     329 -> 346        0.56545
     329 -> 347       -0.27938
     330 -> 347        0.18404
     344 -> 355       -0.11460

 Excited State  91:      Singlet-A      3.1317 eV  395.90 nm  f=0.0113
<S**2>=0.000
     328 -> 346        0.65238
     329 -> 348       -0.17578
     333 -> 348       -0.13400

 Excited State  92:      Singlet-A      3.1390 eV  394.99 nm  f=0.0000
<S**2>=0.000
     327 -> 346        0.22555
     327 -> 347        0.29880
     329 -> 346        0.17436
     329 -> 347        0.49560
     330 -> 346       -0.21534

 Excited State  93:      Singlet-A      3.1403 eV  394.82 nm  f=0.0252
<S**2>=0.000
     328 -> 347        0.64593
     330 -> 348        0.21009
     344 -> 353        0.11305

 Excited State  94:      Singlet-A      3.1454 eV  394.18 nm  f=0.0000
<S**2>=0.000
     320 -> 345        0.32306
     327 -> 346        0.34414
     327 -> 347       -0.18671
     329 -> 347       -0.14152
     330 -> 347       -0.27824
     332 -> 348        0.24310
     344 -> 355        0.16313

 Excited State  95:      Singlet-A      3.1529 eV  393.24 nm  f=0.0000
<S**2>=0.000
     341 -> 351        0.68944

 Excited State  96:      Singlet-A      3.1548 eV  393.00 nm  f=0.0084
<S**2>=0.000
     340 -> 351        0.69784

 Excited State  97:      Singlet-A      3.1586 eV  392.53 nm  f=0.0000
<S**2>=0.000
     318 -> 345       -0.10112
     320 -> 345       -0.18945
```

```
     327 -> 346        0.53794
     328 -> 348        0.15465
     329 -> 346       -0.18500
     330 -> 346        0.13843
     330 -> 347        0.10949
     332 -> 348       -0.11613
     341 -> 351       -0.11538

 Excited State  98:      Singlet-A      3.1658 eV  391.63 nm  f=0.0000
<S**2>=0.000
     318 -> 345       -0.21744
     327 -> 347        0.56644
     329 -> 347       -0.21892
     330 -> 347       -0.11383
     344 -> 354       -0.12237

 Excited State  99:      Singlet-A      3.1688 eV  391.27 nm  f=0.0264
<S**2>=0.000
     319 -> 345        0.41060
     326 -> 346       -0.20843
     332 -> 346       -0.13720
     332 -> 349       -0.14663
     333 -> 348        0.42850

 Excited State 100:      Singlet-A      3.1719 eV  390.88 nm  f=0.0000
<S**2>=0.000
     331 -> 348        0.70056

 Excited State 101:      Singlet-A      3.1729 eV  390.76 nm  f=0.0360
<S**2>=0.000
     314 -> 345        0.10857
     319 -> 345        0.48408
     326 -> 347       -0.10969
     332 -> 347       -0.13229
     332 -> 349        0.13364
     333 -> 348       -0.36919

 Excited State 102:      Singlet-A      3.1771 eV  390.24 nm  f=0.0000
<S**2>=0.000
     318 -> 345        0.60191
     325 -> 346       -0.14808
     325 -> 347       -0.13419
     327 -> 347        0.16586
     332 -> 348       -0.11210
     344 -> 354       -0.10880

 Excited State 103:      Singlet-A      3.1834 eV  389.47 nm  f=0.0000
<S**2>=0.000
     318 -> 345        0.17220
     325 -> 346        0.18497
     328 -> 348        0.10370
     330 -> 347        0.15963
     332 -> 348        0.49383
     333 -> 346       -0.11682
     333 -> 349       -0.19016
     344 -> 355       -0.21670

 Excited State 104:      Singlet-A      3.1954 eV  388.00 nm  f=0.0061
<S**2>=0.000
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     330 -> 348       -0.25678
     343 -> 354        0.28976
     344 -> 353        0.57542

 Excited State 105:      Singlet-A      3.1981 eV  387.68 nm  f=0.0000
<S**2>=0.000
     343 -> 353        0.34170
     344 -> 354        0.58277

 Excited State 106:      Singlet-A      3.2049 eV  386.86 nm  f=0.0099
<S**2>=0.000
     326 -> 346        0.50915
     326 -> 347        0.13316
     330 -> 348       -0.32852
     334 -> 349       -0.12510
     343 -> 354       -0.11439
     344 -> 353       -0.13796

 Excited State 107:      Singlet-A      3.2156 eV  385.57 nm  f=0.1307
<S**2>=0.000
     326 -> 346        0.35495
     328 -> 347       -0.16249
     330 -> 348        0.44405
     343 -> 354        0.13007
     344 -> 356        0.23630

 Excited State 108:      Singlet-A      3.2191 eV  385.15 nm  f=0.0001
<S**2>=0.000
     317 -> 345        0.15080
     318 -> 345        0.10215
     325 -> 346        0.58608
     325 -> 347        0.14913
     332 -> 348       -0.13847
     333 -> 349        0.11729
     335 -> 349       -0.12096

 Excited State 109:      Singlet-A      3.2198 eV  385.06 nm  f=0.0223
<S**2>=0.000
     326 -> 346       -0.14004
     326 -> 347        0.64310

 Excited State 110:      Singlet-A      3.2228 eV  384.70 nm  f=0.0000
<S**2>=0.000
     317 -> 345        0.68301
     325 -> 346       -0.12098
     325 -> 347       -0.11195

 Excited State 111:      Singlet-A      3.2290 eV  383.97 nm  f=0.0001
<S**2>=0.000
     325 -> 346       -0.17460
     325 -> 347        0.64143
     326 -> 348        0.10440

 Excited State 112:      Singlet-A      3.2558 eV  380.81 nm  f=0.0000
<S**2>=0.000
     334 -> 348       -0.11744
     335 -> 349        0.64148
     343 -> 353       -0.19886
```

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 Excited State 113:      Singlet-A      3.2569 eV  380.68 nm  f=0.0038
<S**2>=0.000
     327 -> 348       -0.27383
     329 -> 348       -0.23674
     334 -> 349        0.54190
     343 -> 354       -0.16223

 Excited State 114:      Singlet-A      3.2641 eV  379.84 nm  f=0.0100
<S**2>=0.000
     315 -> 345        0.11559
     316 -> 345       -0.15547
     327 -> 348        0.36138
     329 -> 348        0.33003
     334 -> 349        0.29333
     335 -> 350       -0.15328
     343 -> 354       -0.11938
     344 -> 355        0.19803

 Excited State 115:      Singlet-A      3.2642 eV  379.84 nm  f=0.0016
<S**2>=0.000
     327 -> 348       -0.13965
     328 -> 348       -0.12318
     329 -> 348       -0.12850
     330 -> 347        0.14829
     333 -> 349       -0.13266
     334 -> 349       -0.11191
     342 -> 356        0.17398
     343 -> 352        0.16012
     344 -> 355        0.51080

 Excited State 116:      Singlet-A      3.2660 eV  379.62 nm  f=0.0013
<S**2>=0.000
     314 -> 345       -0.16649
     315 -> 345        0.67348

 Excited State 117:      Singlet-A      3.2704 eV  379.11 nm  f=0.1507
<S**2>=0.000
     316 -> 345        0.51308
     327 -> 348       -0.19469
     329 -> 348        0.21095
     332 -> 349       -0.11265
     334 -> 349        0.10037
     335 -> 350       -0.18985

 Excited State 118:      Singlet-A      3.2784 eV  378.19 nm  f=0.0000
<S**2>=0.000
     328 -> 348       -0.36366
     334 -> 350        0.57784

 Excited State 119:      Singlet-A      3.2800 eV  378.00 nm  f=0.0279
<S**2>=0.000
     316 -> 345        0.24561
     327 -> 348        0.31950
     335 -> 350        0.50529

 Excited State 120:      Singlet-A      3.2901 eV  376.84 nm  f=0.0011
<S**2>=0.000
     324 -> 346        0.24827
     324 -> 347       -0.14198
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     330 -> 348       -0.17636
     344 -> 356        0.57574

 Excited State 121:      Singlet-A      3.2971 eV  376.04 nm  f=0.0106
<S**2>=0.000
     316 -> 345       -0.13152
     324 -> 346        0.11443
     324 -> 347        0.10701
     327 -> 348       -0.19892
     329 -> 348        0.19812
     335 -> 350        0.25107
     342 -> 354        0.15637
     343 -> 355        0.49239

 Excited State 122:      Singlet-A      3.3063 eV  374.99 nm  f=0.0072
<S**2>=0.000
     311 -> 345        0.11402
     313 -> 345        0.68259

 Excited State 123:      Singlet-A      3.3096 eV  374.62 nm  f=0.0001
<S**2>=0.000
     342 -> 353        0.68754

 Excited State 124:      Singlet-A      3.3102 eV  374.56 nm  f=0.0016
<S**2>=0.000
     342 -> 354        0.67991
     343 -> 355       -0.10609

 Excited State 125:      Singlet-A      3.3159 eV  373.91 nm  f=0.0011
<S**2>=0.000
     341 -> 352        0.67961
     342 -> 355       -0.11025

 Excited State 126:      Singlet-A      3.3169 eV  373.79 nm  f=0.0001
<S**2>=0.000
     340 -> 352        0.69685

 Excited State 127:      Singlet-A      3.3186 eV  373.60 nm  f=0.0012
<S**2>=0.000
     314 -> 345        0.31424
     341 -> 352        0.13863
     342 -> 355        0.60022

 Excited State 128:      Singlet-A      3.3232 eV  373.09 nm  f=0.0000
<S**2>=0.000
     326 -> 348        0.37221
     328 -> 348        0.33010
     329 -> 349        0.15164
     333 -> 349        0.24089
     334 -> 350        0.24210
     343 -> 353       -0.17686

 Excited State 129:      Singlet-A      3.3324 eV  372.06 nm  f=0.0458
<S**2>=0.000
     325 -> 348        0.44793
     327 -> 348       -0.11668
     328 -> 349        0.13838
     329 -> 348        0.21991
     332 -> 349       -0.16541
```

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     335 -> 350        0.13259
     343 -> 354       -0.23015
     343 -> 355       -0.22053
     344 -> 353        0.11331
     344 -> 357        0.15197

 Excited State 130:      Singlet-A      3.3354 eV  371.72 nm  f=0.0000
<S**2>=0.000
     326 -> 348       -0.28446
     328 -> 348        0.31348
     329 -> 346        0.10393
     329 -> 349        0.18568
     333 -> 349       -0.16490
     334 -> 350        0.23143
     343 -> 353        0.25632
     343 -> 356        0.19394
     344 -> 354       -0.13423
     344 -> 355        0.11609

 Excited State 131:      Singlet-A      3.3386 eV  371.37 nm  f=0.0784
<S**2>=0.000
     325 -> 348        0.21932
     327 -> 348        0.15846
     328 -> 349       -0.16280
     329 -> 348       -0.22452
     332 -> 349       -0.24762
     335 -> 350       -0.16440
     343 -> 354       -0.23417
     343 -> 355        0.30693
     344 -> 353        0.13450
     344 -> 357       -0.17458

 Excited State 132:      Singlet-A      3.3482 eV  370.30 nm  f=0.0000
<S**2>=0.000
     326 -> 348        0.29030
     332 -> 350        0.13514
     333 -> 349        0.16735
     343 -> 353        0.13690
     343 -> 356        0.53728

 Excited State 133:      Singlet-A      3.3535 eV  369.71 nm  f=0.0427
<S**2>=0.000
     324 -> 346        0.18555
     324 -> 347       -0.14506
     325 -> 348        0.32985
     329 -> 350       -0.12439
     332 -> 349       -0.19241
     333 -> 350       -0.16155
     334 -> 349        0.14832
     343 -> 354        0.37078
     344 -> 353       -0.20251

 Excited State 134:      Singlet-A      3.3568 eV  369.35 nm  f=0.0000
<S**2>=0.000
     326 -> 348        0.22418
     328 -> 350       -0.17069
     335 -> 349        0.14489
     343 -> 353        0.41210
     343 -> 356       -0.33371
```

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     344 -> 354       -0.22041

 Excited State 135:      Singlet-A      3.3767 eV  367.18 nm  f=0.1341
<S**2>=0.000
     314 -> 345        0.21953
     324 -> 346        0.38232
     324 -> 347        0.11793
     330 -> 348        0.10516
     330 -> 350       -0.10233
     333 -> 350        0.42026
     342 -> 355       -0.14333
     344 -> 356       -0.14389

 Excited State 136:      Singlet-A      3.3862 eV  366.15 nm  f=0.0175
<S**2>=0.000
     320 -> 346       -0.10641
     324 -> 346        0.36162
     324 -> 347       -0.33806
     325 -> 348       -0.10019
     329 -> 350        0.13796
     333 -> 350       -0.29286
     343 -> 354       -0.15798
     344 -> 353        0.11402
     344 -> 356       -0.15389

 Excited State 137:      Singlet-A      3.3880 eV  365.95 nm  f=0.0611
<S**2>=0.000
     314 -> 345       -0.13999
     324 -> 346        0.22794
     324 -> 347        0.47976
     328 -> 349       -0.13224
     330 -> 350       -0.24275
     333 -> 350       -0.27458

 Excited State 138:      Singlet-A      3.3944 eV  365.26 nm  f=0.0000
<S**2>=0.000
     319 -> 346       -0.11561
     325 -> 349       -0.10529
     326 -> 348       -0.29621
     332 -> 348        0.18892
     332 -> 350        0.13366
     333 -> 349        0.49335

 Excited State 139:      Singlet-A      3.4023 eV  364.41 nm  f=0.0000
<S**2>=0.000
     319 -> 347       -0.12844
     331 -> 350       -0.12119
     332 -> 350        0.60855
     333 -> 349       -0.14466

 Excited State 140:      Singlet-A      3.4030 eV  364.34 nm  f=0.0000
<S**2>=0.000
     331 -> 349        0.69654

 Excited State 141:      Singlet-A      3.4114 eV  363.44 nm  f=0.0000
<S**2>=0.000
     331 -> 350        0.69029
     332 -> 350        0.10516
```

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 Excited State 142:      Singlet-A      3.4200 eV  362.53 nm  f=0.0081
<S**2>=0.000
     318 -> 346        0.11764
     322 -> 346        0.12297
     325 -> 348        0.24784
     326 -> 349        0.10217
     328 -> 349       -0.10051
     330 -> 350        0.16409
     332 -> 349        0.46897
     333 -> 348        0.14066
     343 -> 355        0.12371
     344 -> 357        0.17566

 Excited State 143:      Singlet-A      3.4221 eV  362.30 nm  f=0.0000
<S**2>=0.000
     321 -> 346        0.10927
     323 -> 346        0.52832
     323 -> 347       -0.28949
     330 -> 349       -0.30346
     332 -> 350       -0.12037

 Excited State 144:      Singlet-A      3.4225 eV  362.27 nm  f=0.0006
<S**2>=0.000
     314 -> 345        0.46537
     315 -> 345        0.12375
     319 -> 345       -0.12500
     333 -> 350       -0.26789
     338 -> 352       -0.11715
     339 -> 349        0.10098
     342 -> 355       -0.26750

 Excited State 145:      Singlet-A      3.4319 eV  361.27 nm  f=0.0000
<S**2>=0.000
     312 -> 345       -0.40327
     323 -> 346        0.21504
     330 -> 349        0.46225
     339 -> 351       -0.16521

 Excited State 146:      Singlet-A      3.4427 eV  360.14 nm  f=0.0191
<S**2>=0.000
     311 -> 345        0.12553
     321 -> 348        0.10230
     322 -> 346        0.63214
     330 -> 350       -0.12023
     344 -> 357       -0.16187

 Excited State 147:      Singlet-A      3.4431 eV  360.10 nm  f=0.0004
<S**2>=0.000
     321 -> 346        0.63127
     322 -> 348        0.12090
     323 -> 346       -0.10230
     323 -> 347        0.10091
     342 -> 356        0.17639

 Excited State 148:      Singlet-A      3.4473 eV  359.65 nm  f=0.0001
<S**2>=0.000
     312 -> 345       -0.24636
     321 -> 346       -0.10512
     321 -> 347       -0.37542
```

```
     323 -> 346        0.15059
     323 -> 347        0.44833
     330 -> 349       -0.16250

 Excited State 149:      Singlet-A      3.4484 eV  359.54 nm  f=0.0371
<S**2>=0.000
     311 -> 345        0.63250
     312 -> 346       -0.16820
     322 -> 346       -0.12506

 Excited State 150:      Singlet-A      3.4495 eV  359.43 nm  f=0.0003
<S**2>=0.000
     311 -> 346       -0.10637
     312 -> 345        0.45199
     321 -> 347       -0.14121
     323 -> 346        0.28328
     323 -> 347        0.19920
     330 -> 349        0.24905
     339 -> 351       -0.19575

 Excited State 151:      Singlet-A      3.4502 eV  359.36 nm  f=0.0048
<S**2>=0.000
     322 -> 347        0.67544
     344 -> 357        0.11038

 Excited State 152:      Singlet-A      3.4547 eV  358.89 nm  f=0.0000
<S**2>=0.000
     309 -> 345       -0.22466
     310 -> 345        0.26351
     319 -> 346       -0.15310
     321 -> 346       -0.19843
     321 -> 347       -0.14136
     323 -> 347       -0.14205
     342 -> 356        0.46847

 Excited State 153:      Singlet-A      3.4581 eV  358.53 nm  f=0.0573
<S**2>=0.000
     322 -> 346        0.16024
     322 -> 347       -0.12507
     328 -> 349       -0.32707
     330 -> 350        0.35198
     332 -> 349       -0.17837
     344 -> 357        0.34366

 Excited State 154:      Singlet-A      3.4639 eV  357.93 nm  f=0.0000
<S**2>=0.000
     321 -> 347        0.52679
     322 -> 348       -0.11360
     323 -> 346        0.14450
     323 -> 347        0.33456
     342 -> 356        0.16215

 Excited State 155:      Singlet-A      3.4833 eV  355.94 nm  f=0.0000
<S**2>=0.000
     324 -> 348        0.52662
     327 -> 349       -0.10826
     328 -> 350        0.37304
     329 -> 349       -0.18302
```

```
 Excited State 156:      Singlet-A      3.4861 eV  355.65 nm  f=0.0000
<S**2>=0.000
     324 -> 348        0.16947
     327 -> 349        0.31600
     328 -> 350        0.15540
     329 -> 349        0.50284
     343 -> 357        0.23180

 Excited State 157:      Singlet-A      3.4914 eV  355.11 nm  f=0.0248
<S**2>=0.000
     320 -> 346        0.11661
     320 -> 347       -0.11767
     327 -> 350        0.32705
     329 -> 350        0.56390

 Excited State 158:      Singlet-A      3.4969 eV  354.55 nm  f=0.0339
<S**2>=0.000
     320 -> 346       -0.21980
     320 -> 347       -0.30839
     324 -> 347        0.17208
     328 -> 349        0.24677
     329 -> 350       -0.11621
     330 -> 350        0.38342
     339 -> 352        0.11349
     344 -> 357       -0.20133

 Excited State 159:      Singlet-A      3.5039 eV  353.85 nm  f=0.0000
<S**2>=0.000
     310 -> 345       -0.11697
     319 -> 346       -0.11370
     327 -> 349        0.56364
     329 -> 349       -0.16342
     343 -> 357       -0.31900

 Excited State 160:      Singlet-A      3.5077 eV  353.46 nm  f=0.0000
<S**2>=0.000
     309 -> 345        0.53616
     310 -> 345        0.45981

 Excited State 161:      Singlet-A      3.5099 eV  353.24 nm  f=0.0000
<S**2>=0.000
     308 -> 345        0.70647

 Excited State 162:      Singlet-A      3.5146 eV  352.77 nm  f=0.0477
<S**2>=0.000
     320 -> 346       -0.29662
     320 -> 347        0.18327
     327 -> 350        0.55781
     329 -> 350       -0.18660

 Excited State 163:      Singlet-A      3.5188 eV  352.35 nm  f=0.0000
<S**2>=0.000
     320 -> 348        0.10378
     324 -> 348       -0.35824
     328 -> 350        0.48049
     339 -> 351       -0.22928
     343 -> 353        0.11666
```

```
 Excited State 164:      Singlet-A      3.5381 eV  350.43 nm  f=0.0004
<S**2>=0.000
     307 -> 345        0.69745

 Excited State 165:      Singlet-A      3.5381 eV  350.42 nm  f=0.0257
<S**2>=0.000
     320 -> 346        0.44404
     323 -> 348       -0.23126
     326 -> 349       -0.22308
     327 -> 350        0.18272
     329 -> 350       -0.22053
     344 -> 357       -0.13220

 Excited State 166:      Singlet-A      3.5430 eV  349.94 nm  f=0.0062
<S**2>=0.000
     318 -> 346       -0.20343
     320 -> 346        0.10351
     320 -> 347       -0.31263
     323 -> 348       -0.18215
     325 -> 350       -0.12983
     326 -> 349        0.31999
     327 -> 350        0.15313
     328 -> 349        0.21245
     329 -> 350       -0.10378
     339 -> 352       -0.12857
     344 -> 357        0.21608

 Excited State 167:      Singlet-A      3.5473 eV  349.51 nm  f=0.0000
<S**2>=0.000
     309 -> 345       -0.19123
     310 -> 345        0.21907
     316 -> 347       -0.11508
     318 -> 348       -0.15204
     319 -> 346        0.35088
     319 -> 347       -0.11984
     325 -> 349       -0.34982
     326 -> 350        0.16034
     339 -> 351       -0.19393

 Excited State 168:      Singlet-A      3.5522 eV  349.04 nm  f=0.0000
<S**2>=0.000
     310 -> 345        0.10251
     316 -> 346       -0.19832
     319 -> 346        0.14352
     319 -> 347       -0.11495
     328 -> 350        0.14581
     330 -> 349        0.21807
     339 -> 351        0.51669
     342 -> 357       -0.13918

 Excited State 169:      Singlet-A      3.5567 eV  348.59 nm  f=0.0118
<S**2>=0.000
     320 -> 346        0.18504
     320 -> 347       -0.20706
     323 -> 348        0.59792

 Excited State 170:      Singlet-A      3.5611 eV  348.16 nm  f=0.0010
<S**2>=0.000
     318 -> 346        0.12610
```

```
     320 -> 346        0.17445
     320 -> 347        0.25305
     321 -> 348        0.15769
     326 -> 349        0.48713
     330 -> 350        0.18171
     339 -> 352        0.15714

 Excited State 171:      Singlet-A      3.5626 eV  348.01 nm  f=0.0003
<S**2>=0.000
     326 -> 350       -0.10685
     342 -> 357        0.65610

 Excited State 172:      Singlet-A      3.5628 eV  347.99 nm  f=0.0264
<S**2>=0.000
     318 -> 347       -0.10298
     320 -> 347        0.20288
     321 -> 348        0.31913
     325 -> 350       -0.24879
     326 -> 349       -0.25476
     328 -> 349        0.32571
     329 -> 348       -0.13462
     344 -> 357        0.16360

 Excited State 173:      Singlet-A      3.5651 eV  347.77 nm  f=0.0000
<S**2>=0.000
     319 -> 347        0.13597
     326 -> 350        0.56632
     342 -> 357        0.14249
     343 -> 357        0.22315

 Excited State 174:      Singlet-A      3.5700 eV  347.30 nm  f=0.0000
<S**2>=0.000
     318 -> 348       -0.15781
     319 -> 346        0.19504
     322 -> 348       -0.13807
     325 -> 349        0.55119
     326 -> 350        0.21595

 Excited State 175:      Singlet-A      3.5766 eV  346.65 nm  f=0.0103
<S**2>=0.000
     321 -> 348        0.15397
     325 -> 350        0.48496
     328 -> 349        0.10382
     340 -> 353        0.12933
     340 -> 354       -0.16692
     341 -> 353        0.36688

 Excited State 176:      Singlet-A      3.5768 eV  346.64 nm  f=0.0078
<S**2>=0.000
     321 -> 348       -0.12112
     325 -> 350       -0.36599
     340 -> 353        0.14303
     340 -> 354       -0.24387
     341 -> 353        0.48156

 Excited State 177:      Singlet-A      3.5771 eV  346.60 nm  f=0.0000
<S**2>=0.000
     340 -> 353       -0.42424
     340 -> 354       -0.17452
```

```
     341 -> 353        0.12528
     341 -> 354        0.50744

 Excited State 178:      Singlet-A      3.5776 eV  346.56 nm  f=0.0002
<S**2>=0.000
     318 -> 348       -0.11607
     319 -> 346        0.12698
     319 -> 347       -0.11017
     322 -> 348        0.35674
     325 -> 349        0.15920
     326 -> 350       -0.20581
     327 -> 349        0.13335
     328 -> 348        0.11154
     329 -> 349       -0.20528
     338 -> 351       -0.12012
     340 -> 353        0.11799
     343 -> 357        0.32286

 Excited State 179:      Singlet-A      3.5805 eV  346.27 nm  f=0.0020
<S**2>=0.000
     340 -> 353        0.46455
     340 -> 354       -0.28692
     341 -> 353       -0.24453
     341 -> 354        0.36069

 Excited State 180:      Singlet-A      3.5812 eV  346.21 nm  f=0.0049
<S**2>=0.000
     340 -> 353        0.21805
     340 -> 354        0.53565
     341 -> 353        0.22958
     341 -> 354        0.30840

 Excited State 181:      Singlet-A      3.5835 eV  345.99 nm  f=0.0050
<S**2>=0.000
     318 -> 346        0.44143
     318 -> 347       -0.20139
     319 -> 348       -0.38255
     320 -> 347       -0.16624
     339 -> 352       -0.14798
     344 -> 357        0.10763

 Excited State 182:      Singlet-A      3.5855 eV  345.79 nm  f=0.0005
<S**2>=0.000
     306 -> 345        0.69891

 Excited State 183:      Singlet-A      3.5867 eV  345.68 nm  f=0.0000
<S**2>=0.000
     305 -> 345        0.70418

 Excited State 184:      Singlet-A      3.5919 eV  345.18 nm  f=0.0000
<S**2>=0.000
     341 -> 355        0.69324

 Excited State 185:      Singlet-A      3.5933 eV  345.04 nm  f=0.0015
<S**2>=0.000
     340 -> 355        0.69945

 Excited State 186:      Singlet-A      3.5958 eV  344.81 nm  f=0.0000
<S**2>=0.000
```

```
     309 -> 345       -0.19949
     310 -> 345        0.23077
     314 -> 346       -0.13797
     318 -> 348        0.14739
     319 -> 346       -0.20240
     322 -> 348        0.36833
     325 -> 349        0.11348
     338 -> 351        0.24219
     342 -> 356       -0.17125

 Excited State 187:      Singlet-A      3.6062 eV  343.81 nm  f=0.0111
<S**2>=0.000
     317 -> 346        0.47344
     317 -> 347        0.25402
     320 -> 347        0.11022
     321 -> 348       -0.35156
     328 -> 349        0.11797

 Excited State 188:      Singlet-A      3.6099 eV  343.45 nm  f=0.0090
<S**2>=0.000
     317 -> 346        0.51869
     317 -> 347       -0.27545
     320 -> 347       -0.11210
     321 -> 348        0.27745
     323 -> 348       -0.10482
     328 -> 349       -0.10519

 Excited State 189:      Singlet-A      3.6153 eV  342.94 nm  f=0.0000
<S**2>=0.000
     309 -> 345        0.14021
     310 -> 345       -0.16261
     314 -> 346        0.13642
     318 -> 348       -0.13943
     319 -> 346        0.11153
     322 -> 348        0.36988
     327 -> 349       -0.12371
     328 -> 348       -0.12699
     329 -> 349        0.19376
     342 -> 356        0.13964
     343 -> 357       -0.28422
     344 -> 355       -0.10078

 Excited State 190:      Singlet-A      3.6170 eV  342.78 nm  f=0.0109
<S**2>=0.000
     317 -> 347        0.59376
     320 -> 347       -0.14388
     321 -> 348        0.26533

 Excited State 191:      Singlet-A      3.6269 eV  341.84 nm  f=0.0046
<S**2>=0.000
     341 -> 356        0.70096

 Excited State 192:      Singlet-A      3.6284 eV  341.71 nm  f=0.0000
<S**2>=0.000
     340 -> 356        0.69037

 Excited State 193:      Singlet-A      3.6334 eV  341.23 nm  f=0.0001
<S**2>=0.000
     316 -> 346        0.10097
```

```
     318 -> 350        0.15843
     319 -> 346       -0.17204
     319 -> 347       -0.39658
     320 -> 348        0.45814
     326 -> 350        0.11562
     340 -> 356       -0.10104

 Excited State 194:      Singlet-A      3.6418 eV  340.44 nm  f=0.0000
<S**2>=0.000
     316 -> 346        0.41894
     316 -> 347       -0.18232
     318 -> 350       -0.11980
     319 -> 346        0.14720
     319 -> 347        0.28792
     320 -> 348        0.28397
     339 -> 351        0.13920

 Excited State 195:      Singlet-A      3.6534 eV  339.37 nm  f=0.0003
<S**2>=0.000
     314 -> 346       -0.14344
     315 -> 346        0.67039
     315 -> 347        0.10183

 Excited State 196:      Singlet-A      3.6569 eV  339.04 nm  f=0.1422
<S**2>=0.000
     316 -> 348        0.13821
     318 -> 346        0.24383
     318 -> 347        0.52713
     319 -> 350       -0.26588
     325 -> 350       -0.12717

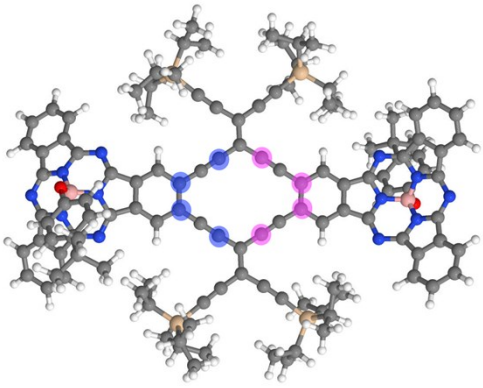
 Excited State 197:      Singlet-A      3.6595 eV  338.80 nm  f=0.0008
<S**2>=0.000
     314 -> 347       -0.13929
     315 -> 346       -0.10257
     315 -> 347        0.67085

 Excited State 198:      Singlet-A      3.6667 eV  338.14 nm  f=0.0000
<S**2>=0.000
     311 -> 347        0.11756
     314 -> 346        0.12563
     316 -> 346        0.25698
     316 -> 347        0.52690
     318 -> 348       -0.17225
     324 -> 350        0.16102
     338 -> 351        0.14138

 Excited State 199:      Singlet-A      3.6935 eV  335.68 nm  f=0.0000
<S**2>=0.000
     313 -> 346        0.68622
     314 -> 346       -0.10661

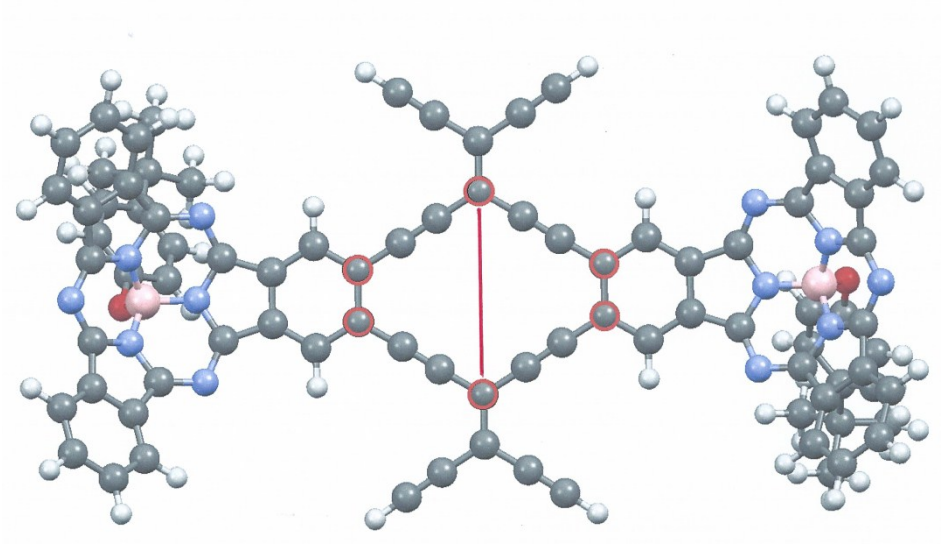
 Excited State 200:      Singlet-A      3.7006 eV  335.04 nm  f=0.0000
<S**2>=0.000
     313 -> 347        0.68798
     314 -> 347       -0.10714
```

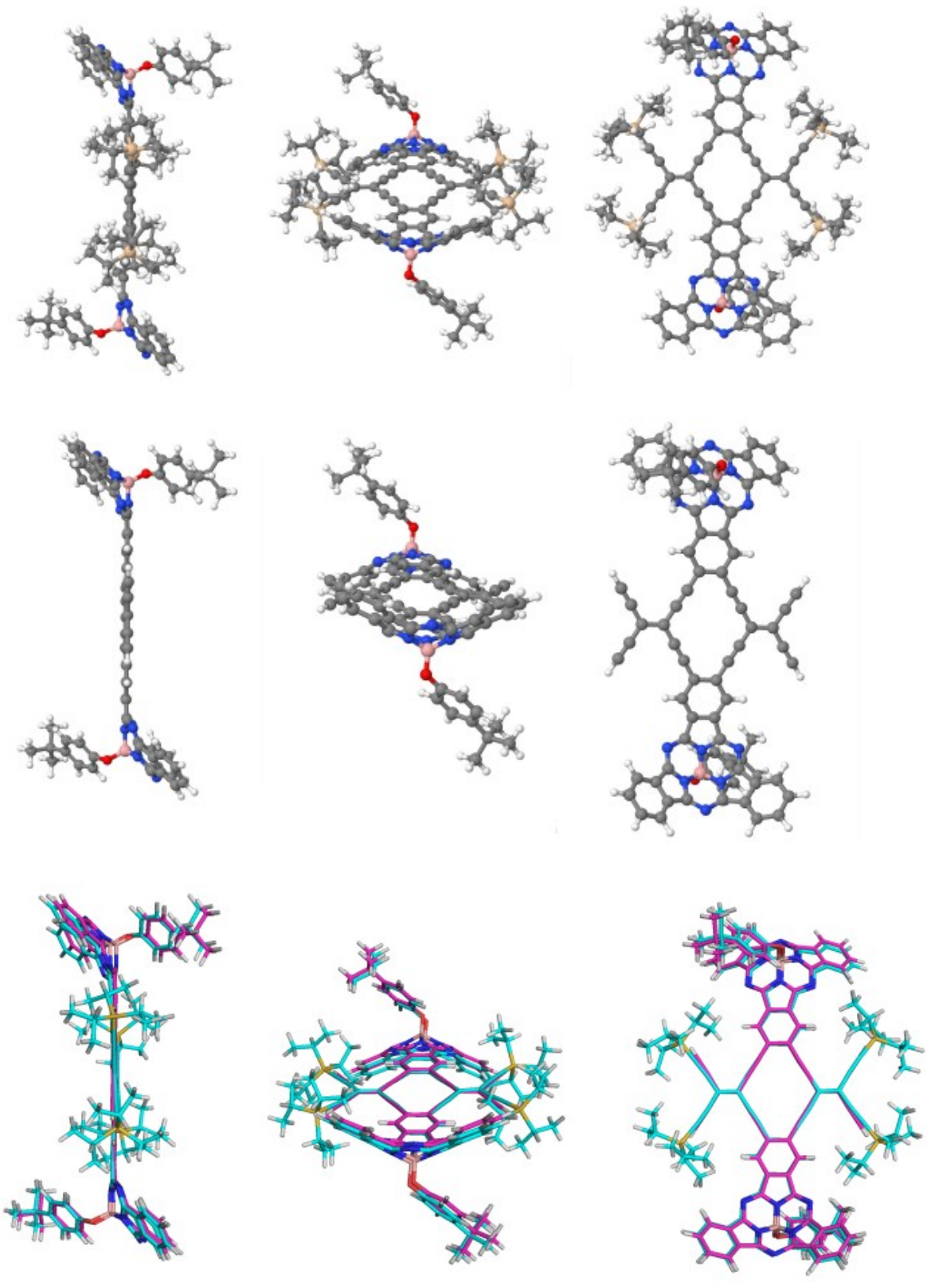
Comparison of RA cores based on calculated structures



On the next page we show a comparison of the central π-syste for structure **4** (with TIPS substituents at the alkyne units) a **4b** (with terminal alkyne units). From these structures it seen that the substitution of TIPS with H only has a limit effect on the degree of planarity of the π-system. To furth quantify this we can compare the angles between two plan defined from the central part of the radiaannulene, indicat with pink and blue dots in the figure to the right. The angle between these planes when the optimization was done with BP86/6-31G(d) came out as 4.43° for **4** and 0.12° for **4b**. Finally, the RMSD (root mean square distance) between the two structures was computed, providing a RMSD = 0.236 Å.

We also determined the deviation from planarity of the central RA system using B3LYP/cc-pVDZ calculations. In the structure shown below, the red line indicates the intersection between the two planes defined by the carbon atoms marked with red circles. The angles between the two planes are: 0.6° for **4a** (with terminal hydrogen atoms instead of TIPS) and 7.4° for **4a-*syn*** (with TIPS groups).





Comparison of π-systems: top: **4** (with TIPS substituents at the alkyne units), middle: **4b** (with terminal alkyne units), bottom: superimposed. For the superimposed structure, the cyan backbone corresponds to **4** and pink to **4b**.

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