**Electronic Supplementary Information for:**

# Photochromic dinuclear iridium(III) complexes having phenoxyl-imidazolyl complexes derivatives

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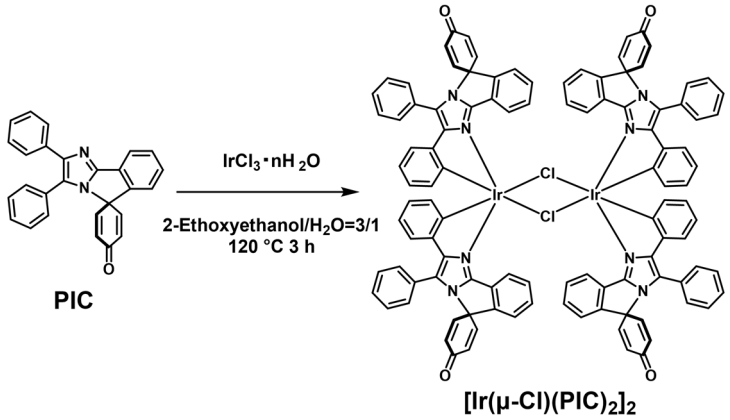
## 1. Syntheses

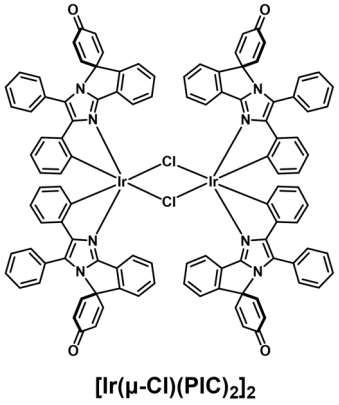
All reactions were monitored by thin-layer chromatography carried out on 0.2 mm E. Merck silica gel plates (60F-254). Column chromatography was performed on silica gel (silica gel 60N, Kanto Chemical Co., Inc.). Proton nuclear magnetic resonance ($^1$H NMR) spectra were recorded at 400 MHz by JNM-ECS 400 MHz (JEOL). High resolution (HR) ESI–TOF–MS spectra were recorded on a Bruker micrOTOF II-AGA1 (Bruker). All reagents were purchased from Tokyo Chemical Industry Co. (TCI), FUJIFILM Wako Pure Chemical Co and Kanto Chemical Co. and were used without further purification. Phenoxyl-imidazolyl radical complexes, **PIC** and **tBu-PIC**, were synthesized according to the literature.[S1] **[Ir(μ-Cl)(2-phenylpyridine)$_2$]$_2$** was synthesized according to the literature.[S2]

**Scheme S1.** Synthesis of **[Ir(μ-Cl)(PIC)$_2$]$_2$.**

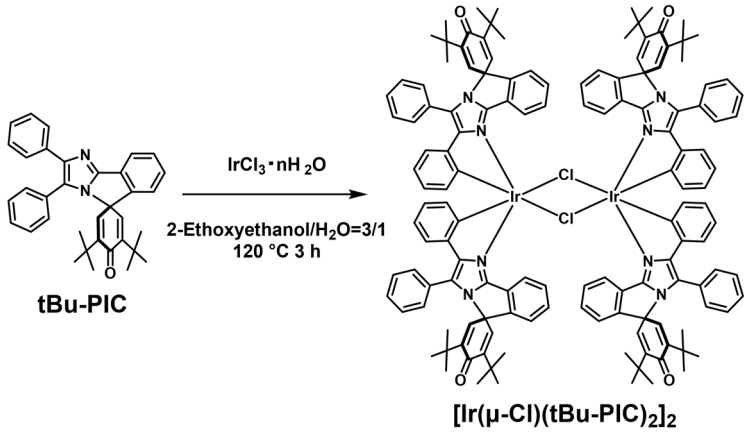



**[Ir(μ-Cl)(PIC)$_2$]$_2$**

A Schlenk flask was charged with **PIC** (120 mg, 0.31 mmol) and iridium(III) chloride hydrate (44 mg, 0.15 mmol) in the solvent pair (6 mL of 2-ethoxyethanol / 2 mL of $H_2O$). The solution was stirred at 120 °C for 3 h. After cooling to room temperature, the reaction mixture was filtered, washed with hexane and $H_2O$. The crude product was purified by recrystallization from $CH_2Cl_2$/hexane to give desired product as pale yellow crystals (84.0 mg, 57%).$^1$H-NMR (400 MHz, $CD_2Cl_2$): δ 9.75 (dd, $J$ = 7.7, 0.9 Hz, 4H), 7.56–7.40 (m, 18H), 7.31-7.22 (m, 16H), 6.71 (d, $J$ = 7.7 Hz, 4H), 6.51–6.40 (m, 8H), 6.24 (dt, $J$ = 9.8, 2.6 Hz, 4H), 6.15 (dd, $J$ = 9.7, 2.0 Hz, 4H), 6.04 (dd, $J$ = 10.0, 1.8 Hz, 4H), 5.91 (d, $J$ = 7.7 Hz, 4H). HRMS (ESI-TOF): calcd. for $[C_{54}H_{34}IrN_4O_2]^+$, 963.2260; found, 963.2309.

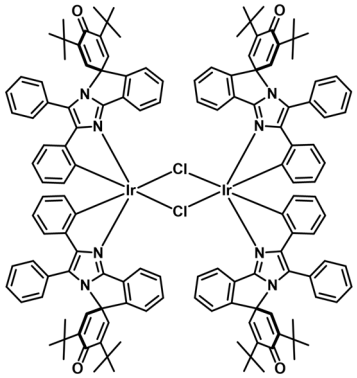


**Scheme S2.** Synthesis of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**.




**[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**

A Schlenk flask was charged with **tBu-PIC** (250 mg, 0.50 mmol) and iridium(III) chloride hydrate (71 mg, 0.24 mmol) in the solvent pair (6 mL of 2-ethoxyethanol/2 mL of $H_2O$). The solution was stirred at 120 °C for 3 h. After cooling to room temperature, the reaction mixture was filtered, washed with hexane and $H_2O$. The crude product was purified by recrystallization from 1,2-dichloroethane/hexane to give desired product as pale-yellow crystals (188 mg, 64%). $^1$H-NMR (400 MHz, $CDCl_3$): δ 9.74 (dd, *J* = 6.8, 1.8 Hz, 4H), 7.44–7.37 (m, 20H), 7.23 (d, *J* = 4.1 Hz, 8H), 6.99 (dd, *J* = 6.6, 2.0 Hz, 4H), 6.61 (dd, *J* = 7.2, 1.4 Hz, 4H), 6.39 (td, *J* = 7.4, 1.1 Hz, 4H), 6.30 (td, *J* = 7.6, 1.5 Hz, 4H), 6.09 (d, *J* = 7.2 Hz, 4H), 5.79 (d, *J* = 2.7 Hz, 4H), 5.52 (d, *J* = 2.7 Hz, 4H), 1.20–1.14 (m, 36H), 0.96 (s, 36H). HRMS (ESI-TOF): calcd. for $[C_{70}H_{66}IrN_4O_2]^+$, 1187.4763; found, 1187.4816.




## 2. Experimental Setups

### X-ray crystallography

Details of the crystal data and a summary of the intensity data collection parameters for **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** are listed in Table S1. A single crystal of **[Ir(μ-Cl)(PIC)$_2$]$_2$** was obtained by vapor diffusion of *n*-hexane into a dichloromethane solution. The data crystal was a yellow prism of approximate dimensions 0.328 mm × 0.258 mm × 0.095 mm. A single crystal of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** was obtained by vapor diffusion of *n*-hexane into a 1,2-dichloroethane solution. The data crystal was a yellow prism of approximate dimensions 0.863 mm × 0.476 mm × 0.222 mm. The data of **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** were collected at 90 K on a

Bruker D8 Venture diffractometer with Mo-Ka radiation (λ = 0.71073 Å) focused by multilayer confocal mirror. All the structures were solved by dual-space method. The structures were refined by a full-matrix least-squares method by using a SHELXL 2014.[S3] In each structure, the non-hydrogen atoms were refined anisotropically. The contribution to the scattering arising from the presence of disordered solvents in the crystal of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** were removed by use of the utility SQUEEZE in the PLATON software package.[S4] CIF files (CCDC2245412−2245413) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

**Steady-State Spectroscopic Measurements**

Absorption spectra were measured on a UV3600 spectrophotometer (Shimazu). The measurements were performed in dichloromethane solutions placed in a 10-mm quartz cell at room temperature after bubbling nitrogen gas to the solution for 10 min.

**Nanosecond-to-Microsecond Transient Absorption Measurements**

Submicrosecond-to-millisecond transient absorption measurements were conducted using a TSP–2000 time resolved spectrophotometer (Unisoku). The second or third harmonics (532 and 355 nm) of a 10 Hz Q–switched Nd:YAG laser (Continuum Minilite II) (ca. 1–2 mJ per 5 ns pulse) were used as the excitation light. Nanosecond transient absorption measurements were conducted by the randomly interleaved-pulse-train (RIPT) method. A picosecond laser, PL2210A (EKSPLA, 1 kHz, 25 ps, 3.4 mJ pulse$^{-1}$ for 355 nm), and a supercontinuum (SC) radiation source (SC-450, Fianium, 20 MHz, pulse width = 50–100 ps depending on the wavelength, 450–2000 nm) were employed as the pump pulse and probe sources, respectively. The wavelength of the excitation pulse was altered 355 nm. The measurements were performed in a dichloromethane solution placed in a 2 mm quartz cell under nitrogen atmosphere while it was stirred at room temperature.

**Femtosecond to Nanosecond Transient Absorption Measurements**

Transient absorption measurements on the femtosecond to nanosecond time scale were conducted by a homemade pump-probe system. An amplified femtosecond laser, Spirit One 1040-8 (Spectra-Physics, 1040 nm, the pulse width: ~270 fs), was split into two beams with a ratio of 1:9. The stronger beam was directed a $\beta$-barium borate (BBO) crystal (Type I, cutting angle = 23.2°) to generate the second harmonic (520 nm) pulse. The fundamental and second harmonic pulses were separated by a dichroic mirror, and the 1040-nm beam passed through a half-wave plate to

align the polarization to parallel to the second harmonic pulse. After passing through a one-directional translational stage, the 1040-nm beam is directed to the BBO crystal (Type I, cutting angle = 32.1°). Alternatively, the 520-nm beam is also directed to the BBO crystal with appropriate time delay and phase matching angle to generate a third harmonic pulse (347 nm), which was used as a pump beam. The pump beam was chopped prior to the sample at 500 Hz for signal differencing. The other weaker beam was focused to a deuterated water placed in a 10-mm quartz cuvette to generate the white light continuum for the probe beam. Both pump and probe beams were focused to the sample solution placed in the 2-mm quartz cuvette. The polarization between the pump and probe pulses was set to the magic angle. The transmitted probe beam was detected with multichannel detection system, PK120-C-RK (UNISOKU), composed of a CMOS linear image sensor and a polychromator. The obtained spectra were calibrated for group velocity dispersion using the data obtained by the optical Kerr signal of $CH_2Cl_2$ between the pump pulse and the white-light continuum. The instrumental response function was shorter than approximately 300 fs. The sample solutions were stirred with a stirrer during the experiments. The measurements were performed at room temperature.

**Picosecond Time-Resolved IR Absorption Measurements**

The fundamental output from a Ti:sapphire regenerative amplifier (Solstice Ace, Spectra Physics, wavelength = 800 nm, repetition rate = 1 kHz, pulse duration = 150 fs) was used to excite two optical parametric amplifiers (TOPAS-C and TOPAS-prime, Light Conversion) and generate a pump UV pulse (wavelength = 355 nm, energy at the sample point = 1 μJ $pulse^{-1}$) and probe IR pulse (spectral coverage = 1360–1700 $cm^{-1}$, <0.4 μJ $pulse^{-1}$). The pump UV pulse was modulated at half of the repetition rate by a mechanical chopper and focused onto the sample noncollinearly against the probe pulse. The probe IR pulse was passed through the photoexcited sample and detected with a 19 cm spectrograph (TRIAX190, HORIBA JOBIN YVON), a multichannel liquid-nitrogen-cooled HgCdTe detector array, and box-car integrators (IR-12-128, InfraRed Associates). The cross-correlation between the pump and probe pulses was estimated to be ~0.5 ps. To remove the artificial signal that appears in transient IR spectra for all time delays, the spectrum at −400 ps, when the probe pulse comes before the pump pulse, was subtracted from all transient IR spectra. **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**, in a $CD_2Cl_2$ solution, was filled into a $CaF_2$ cell (optical path length = 200 μm) and was measured. The accumulation time was 1 h for each time delay and, in total, 18 h for all time delays. Because the sample stage was moved right and left (velocity = 1 mm $s^{-1}$) during the measurement, the transient and steady-state IR spectra of the sample were not changed, even after the experiment was run for 18 h.

## 3. $^1$H NMR spectra

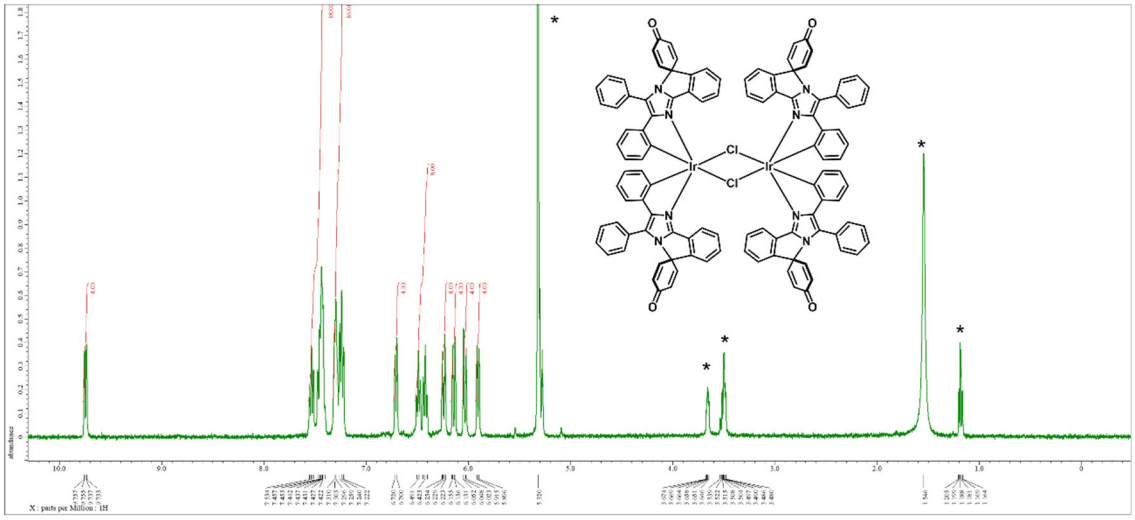


**Fig. S1** $^1$H NMR spectrum of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in $CD_2Cl_2$ (* solvent peaks).

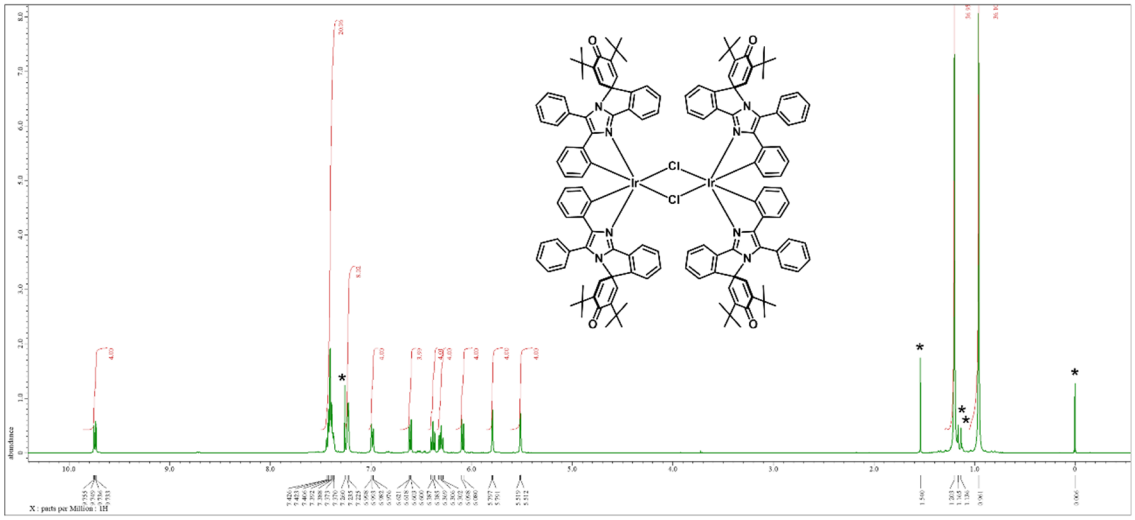


**Fig. S2** $^1$H NMR spectrum of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** in $CDCl_3$ (* solvent peaks).

## 4. HR-ESI-TOF-MS Spectra

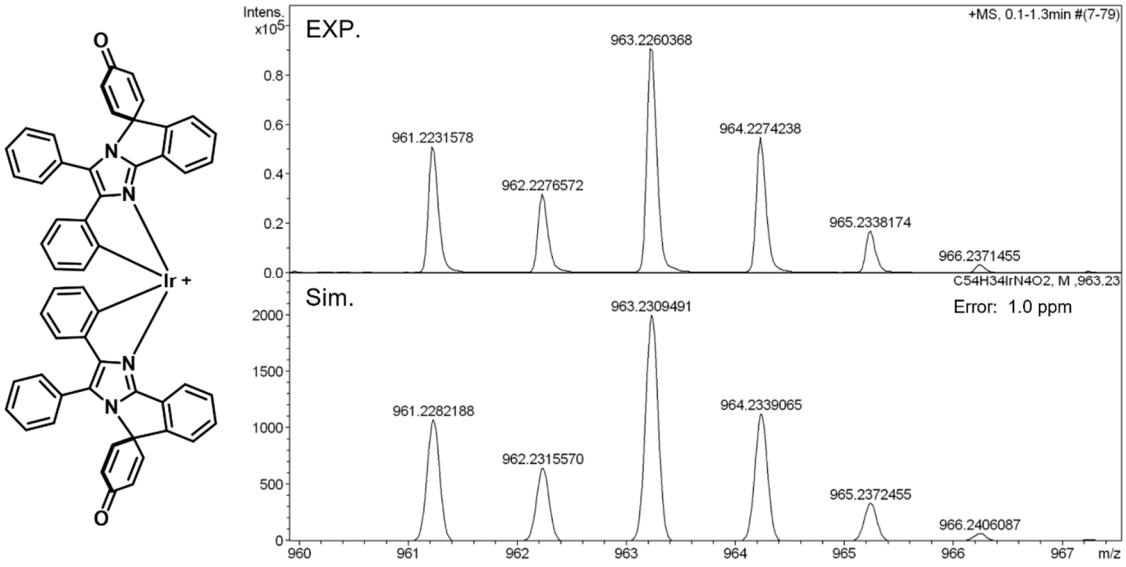



**Fig. S3** HR-ESI-TOF-MS of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

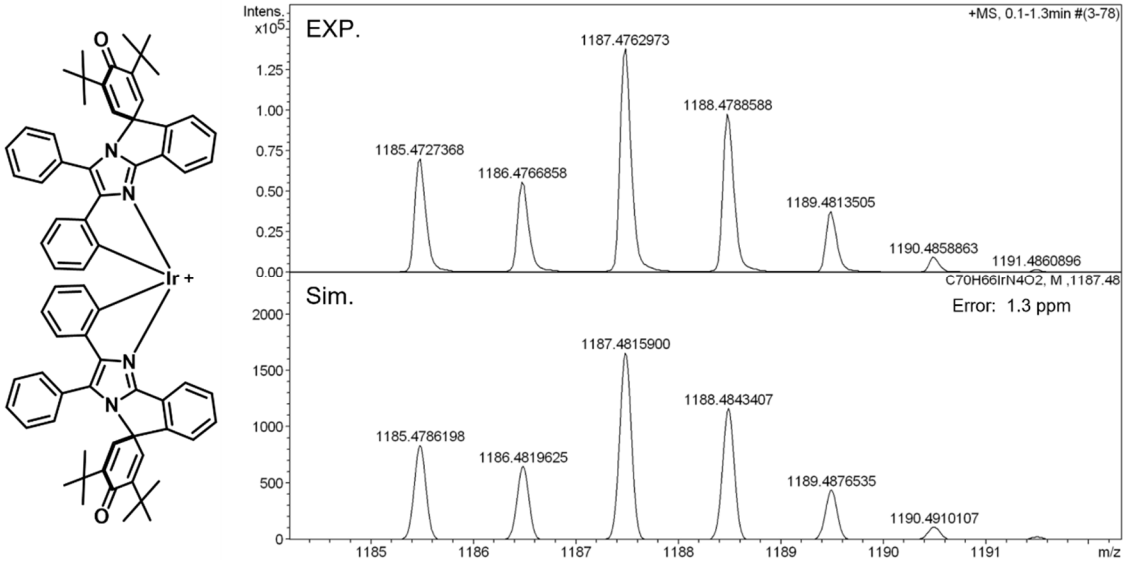



**Fig. S4** HR-ESI-TOF-MS of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**.

## 5. X-ray crystallographic Analyses

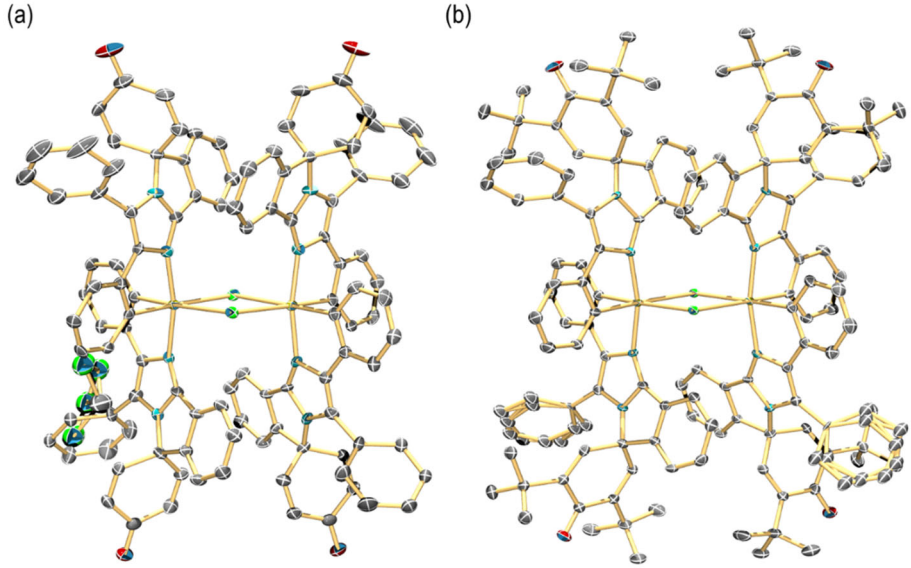



**Fig. S5** X-ray crystal structure (ORTEP view, 50% probability) of (a) **[Ir(μ-Cl)(PIC)$_2$]$_2$** and (b) **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**, where nitrogen, oxygen, iridium and chlorine atoms are highlighted in blue, red, yellow and green respectively. Hydrogen atoms are omitted for clarity.

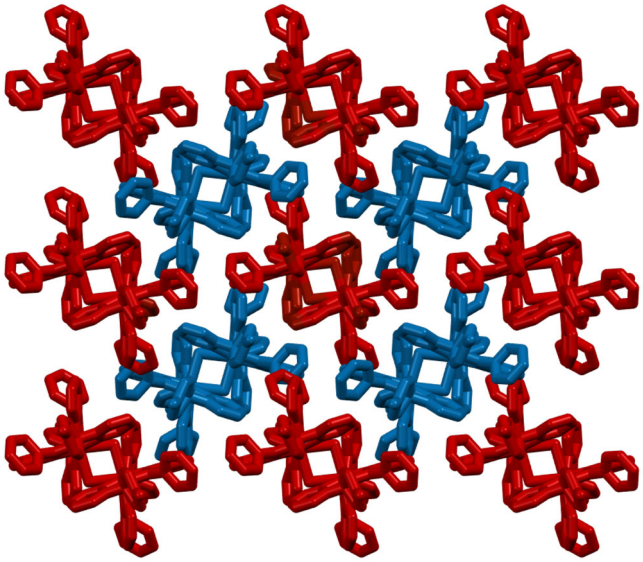


**Fig. S6** Crystal packing diagrams of the crystal structures of **ΔΔ-[Ir(μ-Cl)(PIC)$_2$]$_2$** (red) and **ΛΛ-[Ir(μ-Cl)(PIC)$_2$]$_2$** (blue). Hydrogen atoms are omitted for clarity.

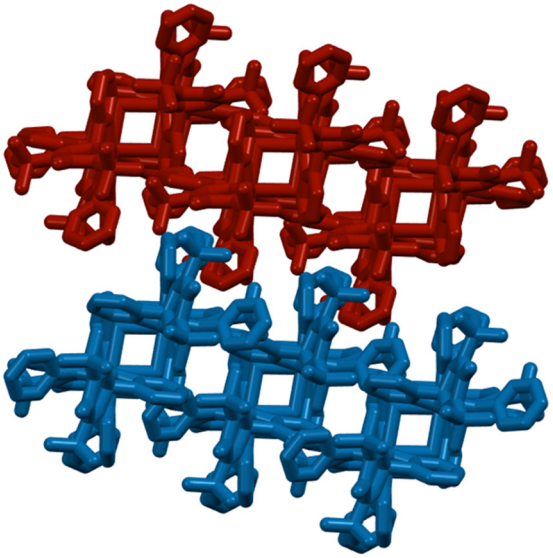


**Fig. S7** Crystal packing diagrams of the crystal structures of ΔΔ-**[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** (red) and ΛΛ-**[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** (blue). Hydrogen atoms are omitted for clarity. One of the disordered structures was shown for clarity.

**Table S1**. Crystallographic Parameters of **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**.

| | **[Ir(μ-Cl)(PIC)$_2$]$_2$** | **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** |
|---|---|---|
| Formula sum | $C_{108}H_{68}Cl_2Ir_2N_8O_4$ | $C_{140}H_{132}Cl_2Ir_2N_8O_4$ |
| Formula weight | 1997.4 | 2445.9 |
| Crystal system | Orthorhombic | Orthorhombic |
| Space group | Fdd2 | C2/c |
| *a* (Å) | 26.0785(8) | 15.7423(3) |
| *b* (Å) | 31.5718(8) | 38.0032(8) |
| *c* (Å) | 22.0025(7) | 24.3288(5) |
| α (deg) | 90 | 90 |
| β (deg) | 90 | 106.201 |
| γ (deg) | 90 | 90 |
| *V* (Å$^3$) | 18115.7(9) | 13976.9(5) |
| *T* (K) | 90 | 90 |
| Z | 8 | 4 |
| $F_{000}$ | 8576.2 | 4992.0 |
| $r_{calcd}$ (g cm$^{-3}$) | 1.586 | 1.162 |
| $R_1$ [I > 2s(I)] | 0.0243 | 0.0209 |
| $wR_2$ [I > 2s(I)] | 0.0806 | 0.0876 |

## 6. Nanosecond to Microsecond Transient Absorption Measurements

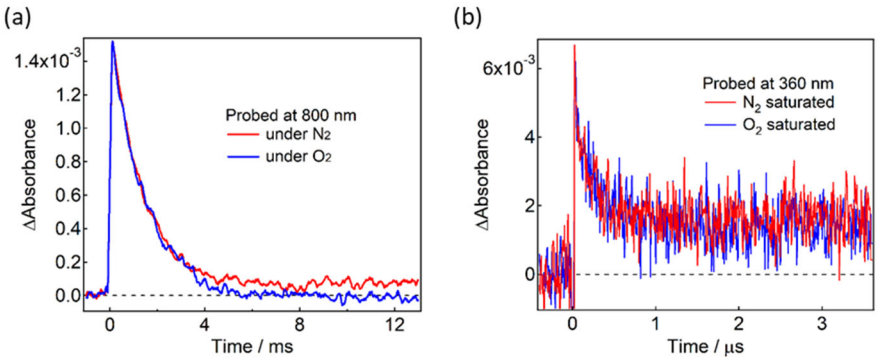



**Fig. S8** Transient absorption dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($2.4 \times 10^{-5}$ M) at room temperature on (a) millisecond and (b) microsecond timescales excited with a 355-nm nanosecond laser pulse (1.0 mJ pulse$^{-1}$) under nitrogen and oxygen atmosphere.

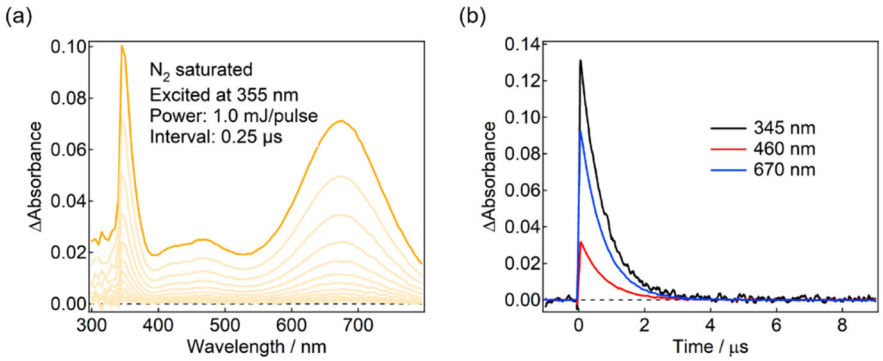



**Fig. S9** (a) Nanosecond to microsecond transient absorption spectra and (b) dynamics of **PIC** in dichloromethane ($7.1 \times 10^{-4}$ M) excited with a 355-nm nanosecond laser pulse (1.0 mJ pulse$^{-1}$) under nitrogen atmosphere at room temperature.

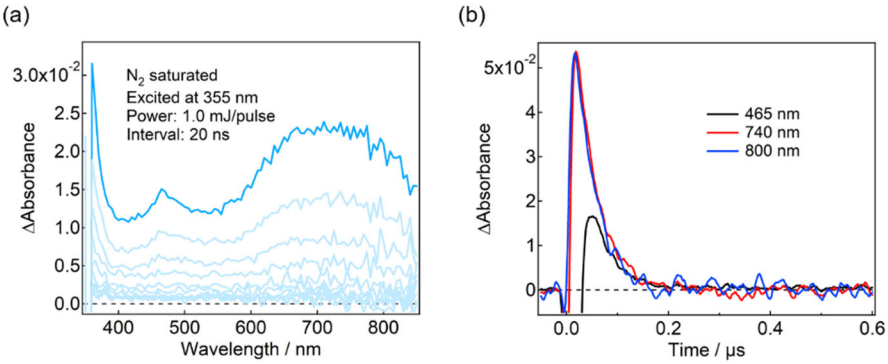



**Fig. S10** (a) Nanosecond to microsecond transient absorption spectra and (b) dynamics of **tBu-PIC** in dichloromethane ($1.1 \times 10^{-3}$ M) excited with a 355-nm nanosecond laser pulse (1.0 mJ pulse$^{-1}$) under nitrogen atmosphere at room temperature.

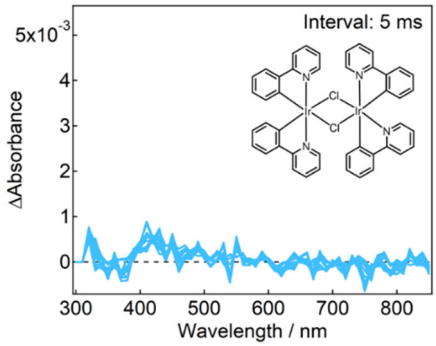



**Fig. S11** Transient absorption spectra of **[Ir(μ-Cl)(2-phenylpyridine)$_2$]$_2$** in dichloromethane ($4.5 \times 10^{-5}$ M) at millisecond time scales excited with a 355-nm nanosecond laser pulse (1.0 mJ pulse$^{-1}$) under nitrogen atmosphere at room temperature.

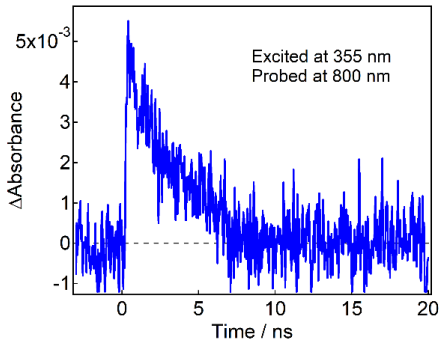



**Fig. S12** Transient absorption dynamics of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** in dichloromethane ($1.2 \times 10^{-4}$ M) excited at 355-nm picosecond laser pulse (3.4 mJ pulse$^{-1}$) under nitrogen atmosphere at room temperature.

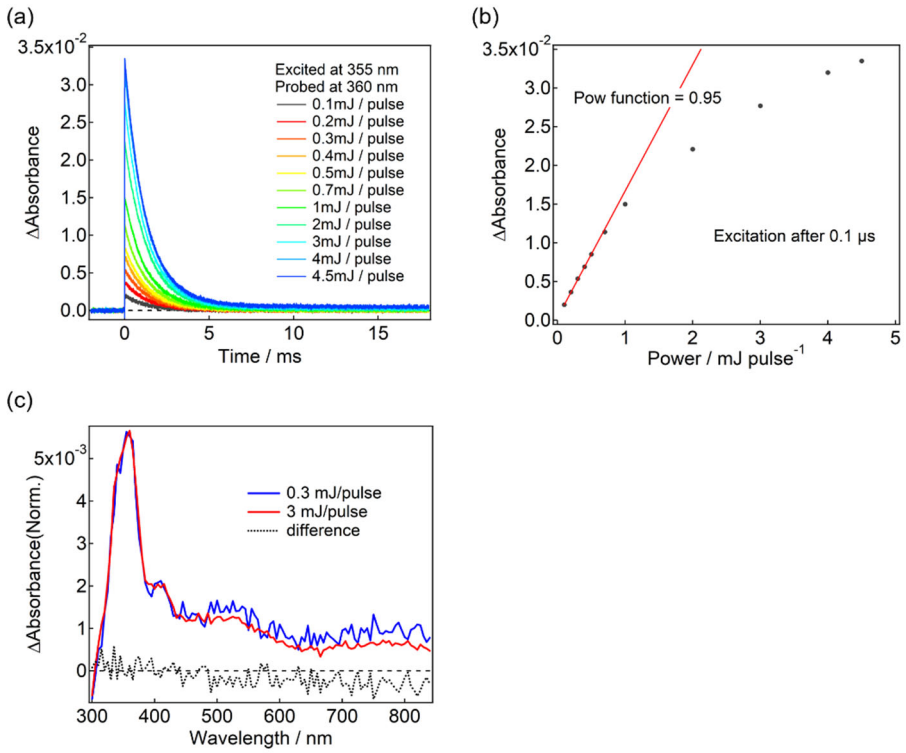



**Fig. S13** (a) Transient absorption dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($2.6 \times 10^{-5}$ M) excited with a 355-nm nanosecond laser pulse with different power under nitrogen atmosphere at room temperature. (b) Plots of excitation light intensity vs. ΔAbsorbances of **[Ir(μ-Cl)(PIC)$_2$]$_2$** after 1 μs of excitation. (c) Normalized transient absorption spectra of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($1.0 \times 10^{-5}$ M) excited with a 355-nm nanosecond laser pulse (0.3 mJ pulse$^{-1}$ (blue) and 3.0 mJ pulse$^{-1}$ (red)) under nitrogen atmosphere at room temperature.

## 7. Kinetics for the Ring-Closing Reaction

**Table S2.** First-order rate constants for the ring-closing reaction of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| T / K | k / $s^{-1}$ |
|---|---|
| 273 | $1.4\times10^2$ |
| 283 | $2.6\times10^2$ |
| 293 | $6.2\times10^2$ |
| 298 | $8.2\times10^2$ |
| 303 | $14\times10^3$ |

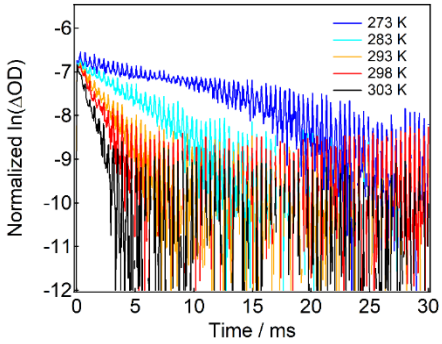



**Fig. S14** First-order kinetic plots of **[Ir(μ-Cl)(PIC)$_2$]$_2$** monitored at 350 nm in dichloromethane ($3.1\times10^{-5}$ M).

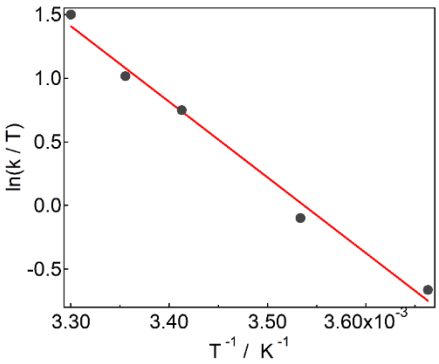



**Fig. S15** Eyring plots for the ring-closing reaction of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($3.1\times10^{-5}$ M).

**Table S3.** Activation parameters for the open−ring isomers of **PIC** in benzene and **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane at 298 K.[S1] Activation enthalpy reflects the change in the thermodynamic stability of the molecule and chemical bonds between the open-ring isomer and the transition state, while activation entropy reflects the change in the molecular structure and environments. The differences in the thermodynamic parameters of **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **PIC** are most probably derived from the coordination bonds between **PIC** and the $Ir^{3+}$ ion. The larger magnitude of the activation entropy may

indicate the steric hindrance by the coordination bonds, *i.e.*, the larger change in the nuclear coordination is necessary for the thermal back reaction. The increase in the activation enthalpy may indicate the interaction between the open-ring isomer and the $Ir^{3+}$ ion.

| | $\Delta G^{\ddagger}$ kJ mol$^{-1}$ | $\Delta H^{\ddagger}$ kJ mol$^{-1}$ | $\Delta S^{\ddagger}$ J mol$^{-1}$ K$^{-1}$ |
|---|---|---|---|
| **PIC** | 36.2 | 31.7 | −14.9 |
| **[Ir(μ-Cl)(PIC)$_2$]$_2$** | 56.2 | 49.4 | −22.7 |

## 8. Subpicosecond-to-nanosecond transient absorption spectra

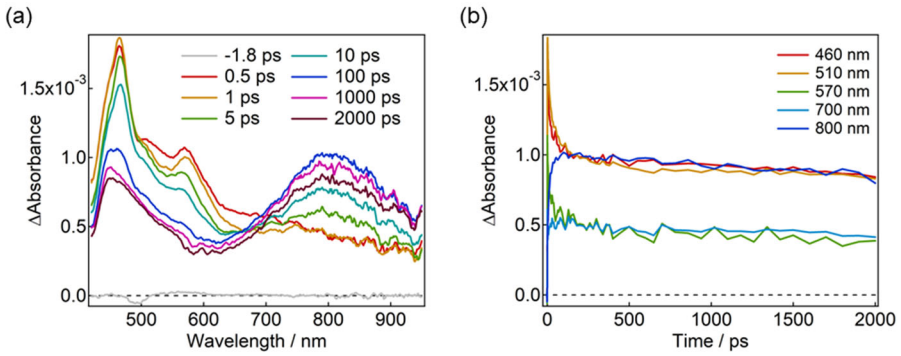



**Fig. S16** Femtosecond to nanosecond transient absorption (a) spectra and (b) dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($1.2 \times 10^{-4}$ M) excited at 347 nm (300 nJ pulse$^{-1}$) at room temperature.

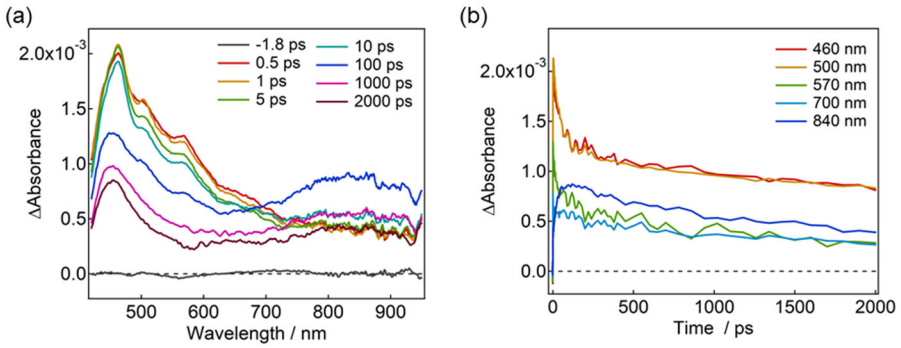



**Fig. S17** Femtosecond to nanosecond transient absorption (a) spectra and (b) dynamics of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** in dichloromethane ($1.5 \times 10^{-4}$ M) excited at 347 nm (300 nJ pulse$^{-1}$) at room temperature.

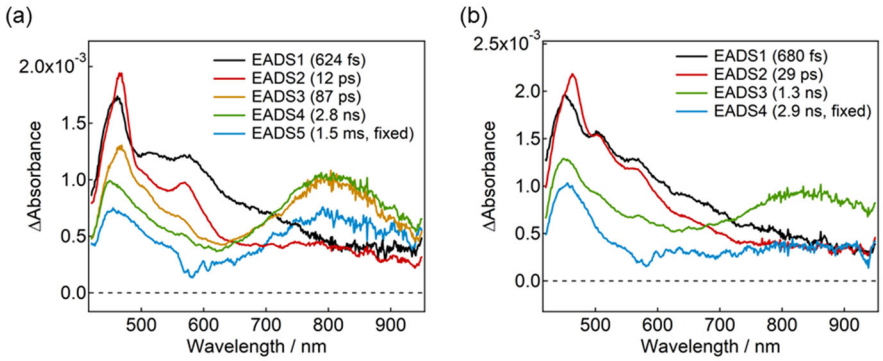



**Fig. S18** EADS of the transient absorption spectra of (a) **[Ir(μ-Cl)(PIC)$_2$]$_2$** and (b) **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** in dichloromethane, respectively.

Global analyses with singular value decomposition (SVD) were performed to elucidate the excited state relaxation pathways.[S5] For **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**, the five-state and four-state sequential kinetic model was assumed to obtain the evolution-associated difference spectra (EADS), and the obtained EADS lifetimes of **[Ir(μ-Cl)(PIC)$_2$]$_2$** and **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** were 624 fs, 12 ps, 87 ps, 2.8 ns and 1.5 ms (fixed) and 680 fs, 29 ps, 1.3 ns and 2.9 ns respectively. The first and second EADS of **[Ir(μ-Cl)(PIC)$_2$]$_2$** (624 fs and 12 ps) reflect bond dissociation to the open-ring isomer. The third EADS (87 ps) is assigned to the structurally unrelaxed open-ring isomer, and the time constant reflects the geometrical relaxation of the open-ring isomer. The time constant of the fourth EADS (2.8 ns) may reflect the thermal back reaction from the open-ring isomer to the initial closed-ring isomer. The time constant concluded that EADS (1.5 ms, fixed) was assigned to the thermal back reaction of the open-ring isomer by flash photolysis. It is noted that it was difficult to obtain the exact time of the fourth EADS (2.8 ns) because of the limitation of the time delay of the experimental setup (up to 2 ns).

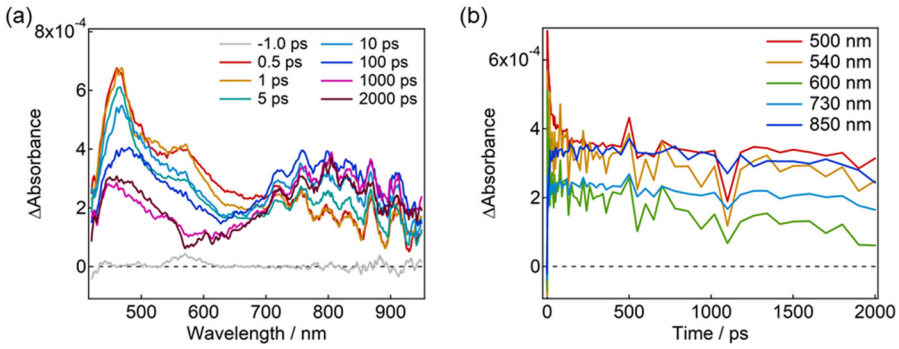



**Fig. S19** Femtosecond to nanosecond transient absorption (a) spectra and (b) dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($4.5 \times 10^{-4}$ M) excited at 410 nm (34 nJ pulse$^{-1}$) at room temperature.

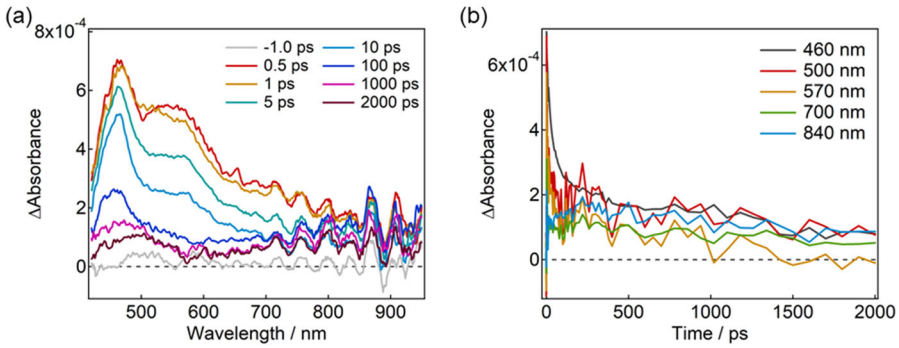



**Fig. S20** Femtosecond to nanosecond transient absorption (a) spectra and (b) dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane ($3.8 \times 10^{-4}$ M) excited at 410 nm (34 nJ pulse$^{-1}$) at room temperature.

## 9. Time-resolved IR Spectra

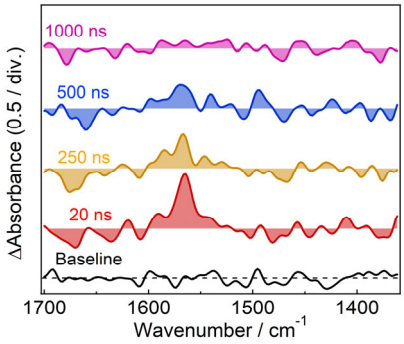



**Fig. S21** Nanosecond time-resolved IR spectra of **PIC** in $CD_2Cl_2$ (~5 × $10^{-3}$ M) excited with a 355-nm nanosecond laser pulse at room temperature.

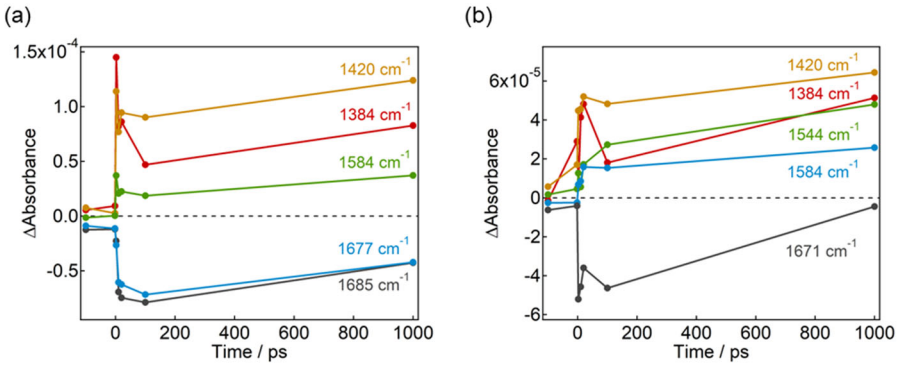



**Fig. S22** Picosecond time-resolved IR dynamics of (a) **[Ir(μ-Cl)(PIC)$_2$]$_2$** and (b) **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** in $CD_2Cl_2$ (~5 × $10^{-3}$ M) excited with a 355-nm femtosecond laser pulse at room temperature.

## 10. Detailed Discussion of the Decay of the Open-Ring Form

The transient absorption dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** have three decay components consisting of nanoseconds, hundreds of nanoseconds, and millisecond timescales after the formation of the open-ring isomer (<100 ps). The origin of the decay is discussed based on the previous reports and simple calculations.

In **PIC** and **PIC** derivatives, the ultrafast bond dissociation processes have been revealed in detail by time-resolved visible and IR spectroscopies and advanced quantum chemical calculations.[S6,S7] After the C−N bond dissociation, a radical pair is generated at the imidazole and phenol moieties, and the spin-spin interaction between them gradually increases with the decrease in the dihedral angle between the two moieties by the reorganization. The generated open-ring isomer has two structural isomers whose biradical characters are different; these are called the biradical and quinoidal forms. The biradical form has two spin states, singlet and triplet biradicals. Transient species generated just after bond dissociation is weighted towards the singlet biradical form. The thermal equilibrium between the two forms (three species including the triplet biradical form) takes hundreds of picoseconds to nanoseconds. The energy gap between the singlet and triplet biradicals is usually very small, and these should exist as the thermal equilibrium. Temperature dependence of electron spin resonance spectroscopy of a **PIC** derivative (**PABI**) shows that the singlet biradical is the ground state in the biradical form.[S8] After the thermal equilibrium, the open-ring isomer decays single-exponentially on timescales of tens of nanoseconds to seconds depending on the molecular structures. The single exponential decay also suggests that the energy gap between singlet and triplet biradicals is small. On the other hand, in a **PIC** derivative whose spin-spin interaction between the imidazolyl and phenoxyl radicals is relatively weak,[S9] the thermal equilibrium between the biradical and quinoidal forms are substantially decelerated and is observed in hundreds of nanoseconds, whereas the thermal back reaction occurs on millisecond timescales. Considering these previous results, the **PIC**-coordinated $Ir^{3+}$ complex also exhibits similar dynamic properties after the bond breaking. Namely, at least the two decay components, the thermal equilibrium between biradical and quinoidal forms and the thermal back reactions to the close-ring isomer, are expected to be observed in the **PIC**-coordinated $Ir^{3+}$ complexes.

The transient absorption dynamics of **[Ir(μ-Cl)(PIC)$_2$]$_2$** have three decay components consisting of nanoseconds, hundreds of nanoseconds, and millisecond timescales after the formation of the open-ring isomer (<100 ps). The decay on millisecond timescales can be assigned to the thermal back reaction from the open-ring isomer (the thermal equilibrium between the biradical and quinoidal forms) to the close-ring isomer. The triplet biradical form would not be the origin of the millisecond transient species because the S-T gap of biradicals should be very small and cannot account for the millisecond decay. Time-resolved IR measurements show that the IR band at ~1550 $cm^{-1}$ gradually increases on a timescale of hundreds of picoseconds to nanoseconds despite the gradual decrease in

the visible transient absorption signals associated with the open-ring isomer. This may indicate that the thermal equilibrium between the biradical and quinoidal forms occurs on hundreds of picoseconds to nanosecond timescales. However, it was difficult to dictate the origin of the decay on hundreds of nanosecond timescales. It may be originated from the fast thermal back reaction to the close-ring isomer due to the steric hindrance or electronic interaction by the $Ir^{3+}$ ion because the signal associated with the open-ring isomer of **[Ir(μ-Cl)(PIC)$_2$]$_2$** is substantially smaller than that of **PIC**.

The triplet excited state of the close-ring isomer can be excluded from the origin of these decays because the decay process from nanosecond to millisecond did not depend on the molecular oxygen at all (Fig. S8).

Moreover, the multiphoton process can be also excluded from our experiments by the following calculations. The characteristics of the excitation pulse are as below: wavelength = 347 nm, pulse duration = ~300 fs, intensity = 300 nJ/pulse, FWHM of the beam spot = 300 μm (measured by the knife-edge method). Using these parameters, the number of photons per pulse can be calculated as $5.2 \times 10^{11}$ photons pulse$^{-1}$. The molar absorption coefficient of **[Ir(μ-Cl)(PIC)$_2$]$_2$** at the excitation wavelength (347 nm) is $7.4 \times 10^4$ M$^{-1}$ cm$^{-1}$. The molar absorption coefficient can be converted to the absorption cross section ($1.2 \times 10^{-16}$ cm$^2$). By multiplying the number of photons per pulse by the absorption cross section, we can estimate the number of photons supplied to one molecule under the excitation condition. The value is 0.08 photons/molecule, indicating that no nonlinear optical processes occur under the excitation condition. Therefore, we can safely exclude the effect of the multiphoton processes on the transient absorption dynamics.

## 10. DFT calculations

All calculations were carried out using the Gaussian 09 program (Revision D.01).[S10] The molecular structure was fully optimized at the B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of theory, and the analytical second derivative was computed using vibrational analysis to confirm each stationary point to be a minimum. TDDFT calculations were performed at the B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory for the optimized structures.

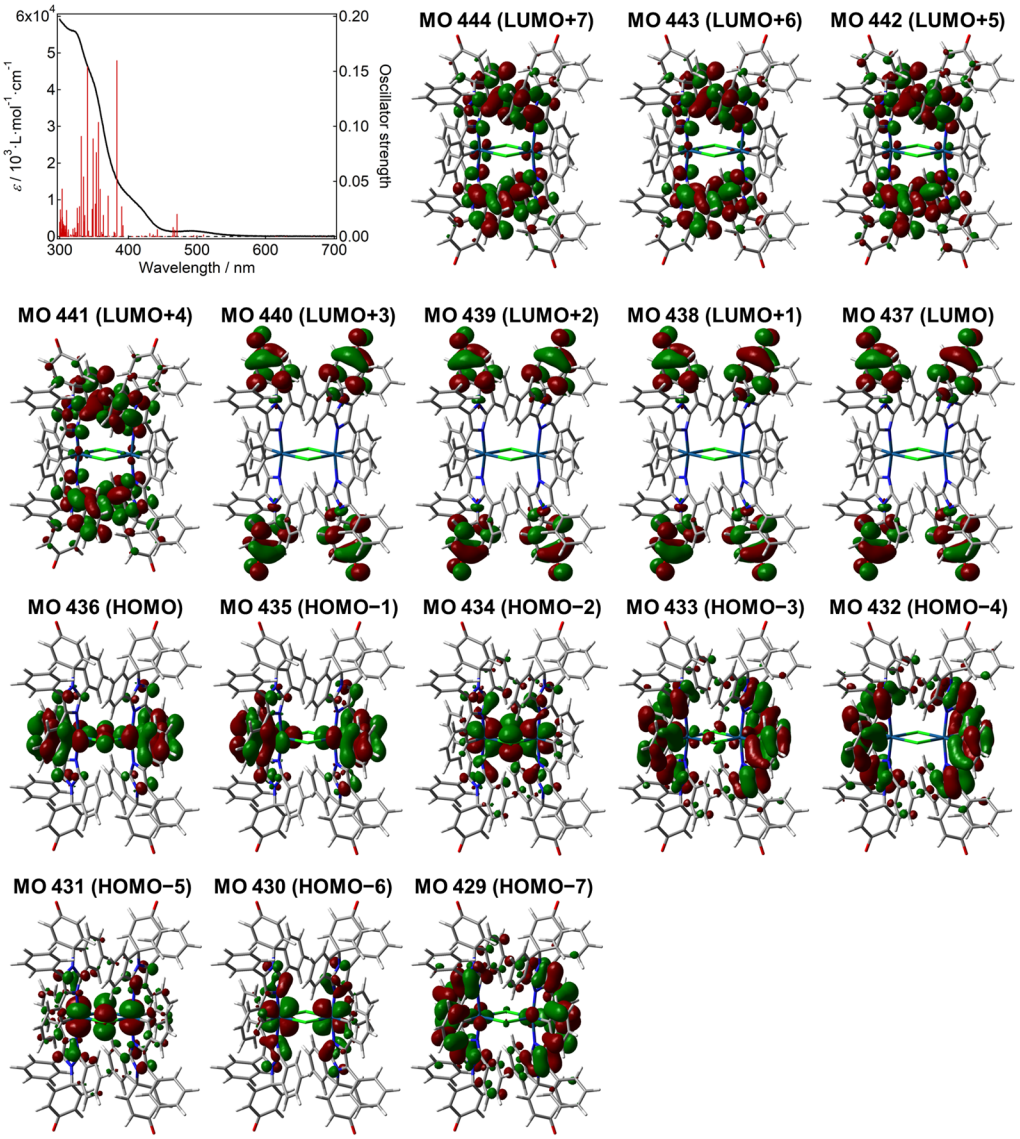



**Fig. S23** UV-vis absorption spectrum of **[Ir(μ-Cl)(PIC)$_2$]$_2$** in dichloromethane at room temperature. The calculated absorption spectrum B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir]// B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory is shown by the red vertical lines. The relevant molecular orbitals of the **[Ir(μ-Cl)(PIC)$_2$]$_2$** calculated at the B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory.

**Table S4.** Selected calculated electronic transition of **[[Ir(μ-Cl)(PIC)$_2$]$_2$** at the B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level.

| No. | Wavelength (nm) | Coefficients | Electronic Transition | | | *f* |
|---|---|---|---|---|---|---|
| 1 | 509.73 | 0.10020 | 429 HOMO-7 | → | 438 LUMO+1 | 0.0015 |
| | | 0.11913 | 432 HOMO-4 | → | 439 LUMO+2 | |
| | | 0.12710 | 433 HOMO-3 | → | 437 LUMO | |
| | | 0.66854 | 434 HOMO-2 | → | 437 LUMO | |
| 2 | 470.92 | -0.24741 | 435 HOMO-1 | → | 444 LUMO+7 | 0.0202 |
| | | 0.65216 | 436 HOMO | → | 442 LUMO+5 | |
| 3 | 383.35 | -0.27963 | 434 HOMO-2 | → | 441 LUMO+4 | 0.1597 |
| | | 0.11279 | 435 HOMO-2 | → | 444 LUMO+7 | |
| | | -0.37277 | 435 HOMO-1 | → | 445 LUMO+8 | |
| | | 0.44604 | 436 HOMO | → | 446 LUMO+9 | |
| | | -0.16327 | 436 HOMO | → | 449 LUMO+12 | |
| 4 | 340.53 | 0.63832 | 430 HOMO-6 | → | 443 LUMO+6 | 0.1542 |
| | | 0.15598 | 431 HOMO-5 | → | 444 LUMO+7 | |
| | | -0.10510 | 433 HOMO-3 | → | 441 LUMO+4 | |

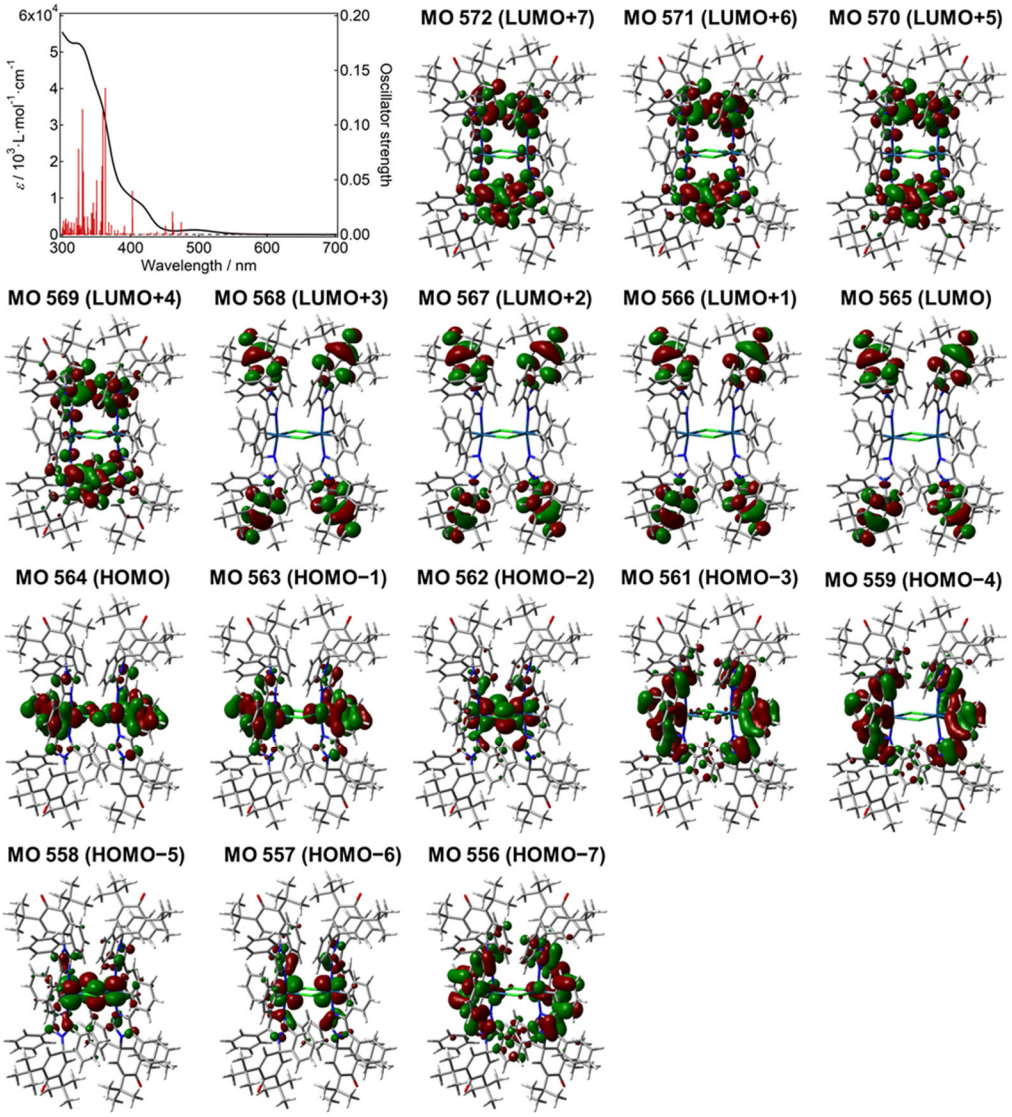



**Fig. S24** UV-vis absorption spectrum of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** in dichloromethane at room temperature. The calculated absorption spectrum B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir]// B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory is shown by the red vertical lines. The relevant molecular orbitals of the **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** calculated at the B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory.

**Table S5.** Selected calculated electronic transition of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** at the B3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level.

| No. | Wavelength (nm) | Coefficients | Electronic Transition | | | *f* |
|---|---|---|---|---|---|---|
| 1 | 580.23 | -0.23547 | 563 HOMO-1 | → | 566 LUMO+1 | 0.0001 |
| | | -0.19623 | 563 HOMO-1 | → | 568 LUMO+3 | |
| | | 0.62616 | 564 HOMO | → | 568 LUMO+3 | |
| 2 | 474.01 | -0.10224 | 562 HOMO-2 | → | 566 LUMO+1 | 0.0111 |
| | | 0.16194 | 563 HOMO-1 | → | 571 LUMO+6 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | 0.67169 | 564 HOMO | → | 569 LUMO+4 | |
| 3 | 461.30 | -0.11730 | 562 HOMO-2 | → | 568 LUMO+3 | 0.0206 |
| | | -0.17249 | 563 HOMO-1 | → | 572 LUMO+7 | |
| | | 0.66454 | 564 HOMO | → | 570 LUMO+5 | |
| 4 | 402.58 | 0.15791 | 557 HOMO-7 | → | 565 LUMO | 0.0398 |
| | | -0.30972 | 558 HOMO-6 | → | 567 LUMO+2 | |
| | | 0.57230 | 562 HOMO-2 | → | 569 LUMO+4 | |
| 5 | 362.96 | 0.45082 | 560 HOMO-4 | → | 571 LUMO+6 | 0.1337 |
| | | 0.18492 | 560 HOMO-4 | → | 572 LUMO+7 | |
| | | -0.14183 | 561 HOMO-3 | → | 569 LUMO+4 | |
| | | 0.11243 | 561 HOMO-3 | → | 570 LUMO+5 | |
| | | -0.27002 | 563 HOMO-1 | → | 573 LUMO+8 | |
| | | -0.26009 | 564 HOMO | → | 574 LUMO+9 | |
| | | -0.13465 | 564 HOMO | → | 578 LUMO+13 | |
| 6 | 329.55 | -0.25936 | 555 HOMO-9 | → | 569 LUMO+4 | 0.1143 |
| | | -0.10067 | 555 HOMO-9 | → | 570 LUMO+5 | |
| | | -0.11312 | 556 HOMO-8 | → | 569 LUMO+4 | |
| | | 0.47990 | 557 HOMO-7 | → | 571 LUMO+6 | |
| | | -0.11945 | 558 HOMO-6 | → | 570 LUMO+5 | |
| | | -0.10637 | 559 HOMO-5 | → | 572 LUMO+7 | |
| | | 0.13643 | 563 HOMO-1 | → | 577 LUMO+12 | |
| | | 0.11132 | 563 HOMO-1 | → | 581 LUMO+16 | |
| | | 0.17347 | 564 HOMO | → | 582 LUMO+17 | |
| | | -0.15252 | 564 HOMO | → | 583 LUMO+18 | |

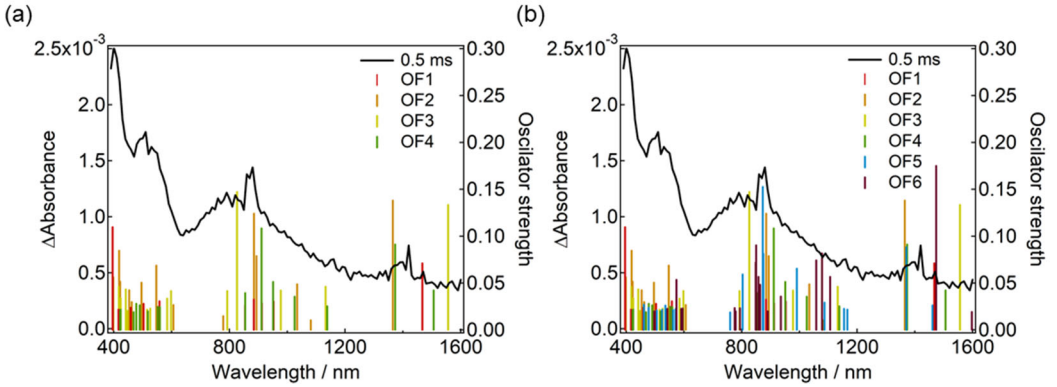



**Fig. S25** Transient absorption spectra of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$** at 0.5 ms (black line) after excitation in dichloromethane at room temperature. Vertical lines indicate the theoretical spectra of (a) open-ring isomers (OF1–OF4) and (b) open-ring isomers (OF1–OF6) (UB3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir]// UB3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory).

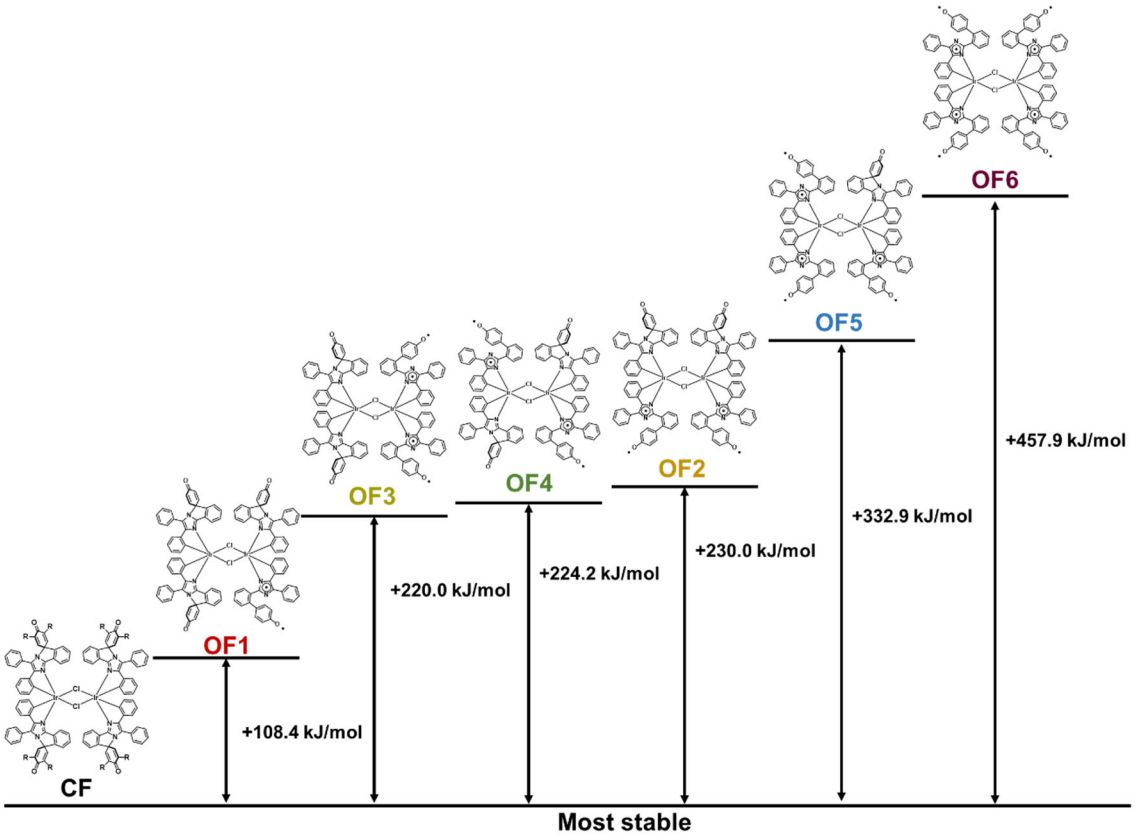



**Fig. S26** Relative energy of closed-ring isomer and the possible open-ring isomers of **[Ir(μ-Cl)(PIC)$_2$]$_2$** calculated at the UB3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory.

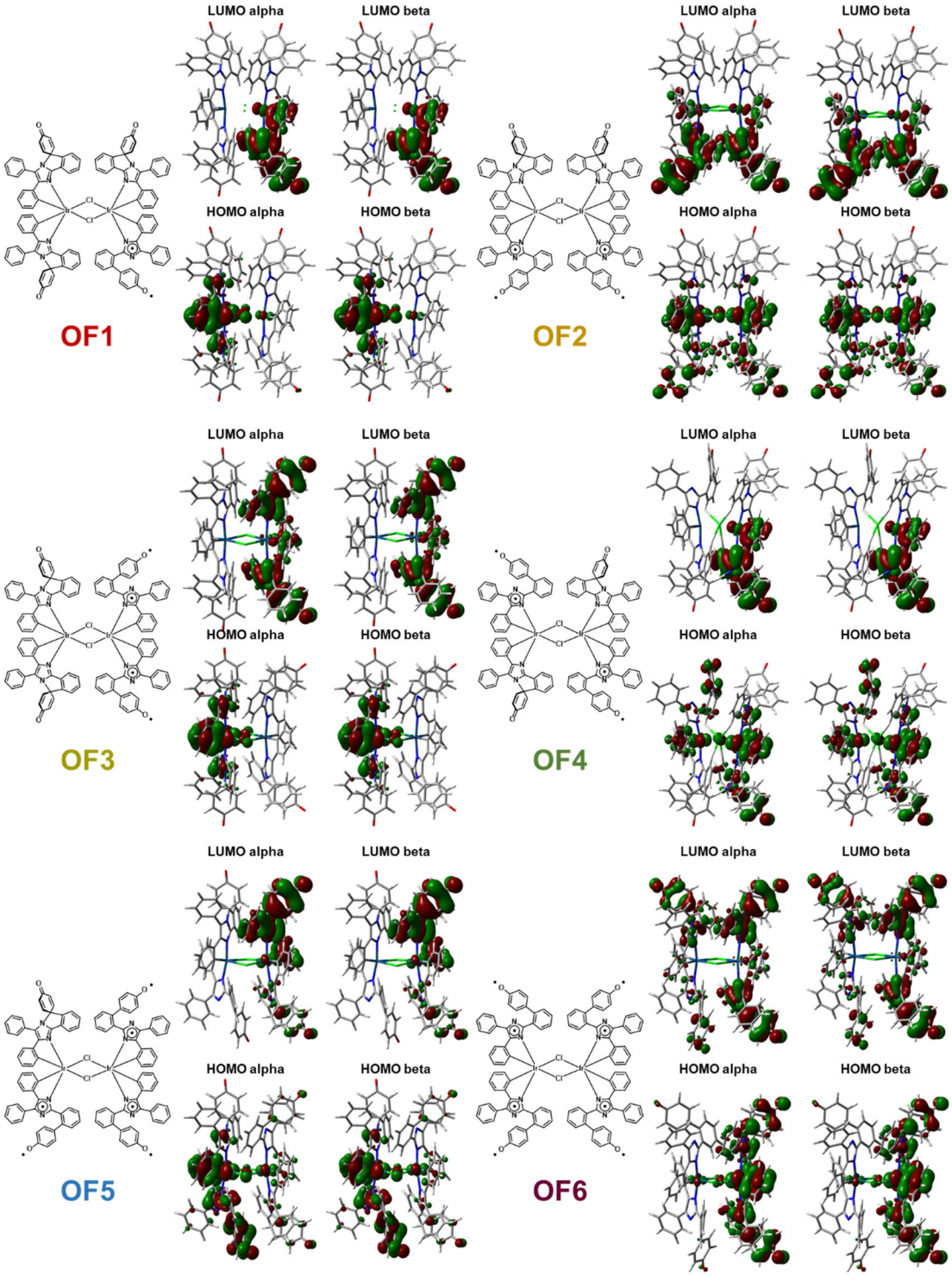



**Fig. S27** The relevant molecular orbitals of the possible open-ring isomers of **[Ir(μ-Cl)(PIC)$_2$]$_2$** calculated at UB3LYP/6-31G[C H N O Cl]/LANL2DZ[Ir] level of the theory.

**Table S6.** Standard orientation of the optimized geometry for the closed-ring isomer of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | 0.002235 | 2.10252 | 0.001335 |
| C | 0.068166 | 3.458041 | -1.50045 |
| C | 6.71318 | 2.338744 | 0.45859 |
| C | -6.70784 | 2.344271 | -0.46047 |
| N | -4.23999 | 2.745517 | -0.4116 |
| Cl | 0.00065 | -1.3E-05 | 1.68163 |
| C | -3.80899 | 1.411108 | 1.415913 |
| N | -2.05671 | 2.325491 | -0.35133 |
| N | 2.061597 | 2.323194 | 0.353796 |
| N | 4.24527 | 2.741599 | 0.413029 |
| O | 9.187823 | 4.781184 | -0.44007 |
| O | -9.18119 | 4.789727 | 0.434397 |
| C | -3.23445 | 2.049572 | 0.2368 |
| C | -5.16768 | 1.809333 | 1.489033 |
| C | -2.33145 | 3.227218 | -1.40758 |
| C | 1.188529 | 3.761046 | 2.113816 |
| C | 3.238842 | 2.04656 | -0.23502 |
| C | -5.52499 | 2.798581 | 0.349017 |
| C | 2.337512 | 3.224766 | 1.409842 |
| C | 1.211506 | 4.056147 | -2.06173 |
| C | -1.18172 | 3.763925 | -2.11007 |
| C | 5.170846 | 1.806231 | -1.48903 |
| C | 3.812032 | 1.40865 | -1.41506 |
| C | 5.529585 | 2.794813 | -0.34894 |
| C | 3.274533 | 0.574966 | -2.40025 |
| C | -1.20472 | 4.053642 | 2.06791 |
| C | 5.993208 | 1.385859 | -2.52526 |
| C | -3.27255 | 0.57684 | 2.401203 |
| C | -4.1061 | 0.153657 | 3.446047 |
| C | -5.69229 | 4.174775 | 0.947937 |
| C | -0.0619 | 3.456287 | 1.504728 |
| C | 5.696942 | 4.171519 | -0.94642 |
| C | 7.904434 | 2.976937 | 0.469232 |
| C | 1.132246 | 4.86665 | -3.20112 |
| C | -3.69221 | 3.501761 | -1.44548 |
| C | -5.99091 | 1.389169 | 2.524646 |
| C | 3.698549 | 3.49833 | 1.447121 |
| C | 9.115255 | 2.46938 | 1.282588 |
| C | -7.89826 | 2.983955 | -0.47287 |
| C | 4.107103 | 0.151792 | -3.44586 |
| C | -6.85439 | 4.857349 | 0.974293 |
| C | 6.859687 | 4.853046 | -0.97381 |
| C | 8.059962 | 4.238091 | -0.32831 |
| C | -4.47858 | 4.400378 | -2.31691 |
| C | 5.450308 | 0.5477 | -3.51354 |
| C | 4.48556 | 4.398668 | 2.315913 |
| C | -0.10085 | 5.108673 | -3.81717 |
| C | -1.12442 | 4.862126 | 3.208662 |
| C | 0.109187 | 5.102725 | 3.824272 |
| C | -5.44915 | 0.550245 | 3.51292 |
| C | -8.05406 | 4.244458 | 0.325748 |
| C | -1.25921 | 4.559541 | -3.26638 |
| C | 1.267023 | 4.554407 | 3.271606 |
| C | 8.753344 | 1.21242 | 2.106287 |
| C | 10.28619 | 2.098297 | 0.328288 |
| C | 4.349638 | 5.79554 | 2.19636 |
| C | 5.360843 | 3.881287 | 3.288719 |
| C | -6.98626 | 6.238726 | 1.650612 |
| C | -5.34395 | 3.880218 | -3.2971 |
| C | 9.584617 | 3.568476 | 2.278588 |
| C | -10.2805 | 2.104679 | -0.33768 |
| C | -7.50235 | 7.284991 | 0.62254 |
| C | 5.950797 | 6.128284 | 3.98738 |
| C | 5.077269 | 6.653158 | 3.026729 |
| C | -9.108 | 2.478372 | -1.28902 |
| C | 6.992107 | 6.235228 | -1.64848 |
| C | 6.088569 | 4.741456 | 4.118136 |
| C | 5.628779 | 6.735043 | -2.18311 |
| C | -4.35111 | 5.797609 | -2.19348 |
| C | -7.97037 | 6.149135 | 2.851893 |
| C | -8.74426 | 1.223254 | -2.11469 |
| C | -9.57553 | 3.579971 | -2.2834 |
| C | -5.62325 | 6.735614 | 2.18832 |
| C | 7.974064 | 6.145905 | -2.8515 |
| C | 7.512048 | 7.279052 | -0.61957 |
| C | -5.07734 | 6.653045 | -3.02738 |
| C | -6.07022 | 4.738164 | -4.13012 |
| C | -5.94087 | 6.125477 | -3.9955 |
| Ir | -0.00245 | -2.10149 | 0.000216 |
| C | 0.061418 | -3.45588 | 1.503049 |
| C | 6.70686 | -2.34606 | -0.46124 |
| C | -6.7135 | -2.33959 | 0.458231 |
| N | -4.24557 | -2.74054 | 0.411569 |
| Cl | 0.000423 | 0.000928 | -1.68069 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.81288 | -1.40769 | -1.41658 | C | 1.259846 | -4.56021 | -3.2662 |
| N | -2.06197 | -2.32156 | 0.352482 | C | 8.741908 | -1.23154 | -2.12314 |
| N | 2.056535 | -2.32508 | -0.35186 | C | 10.28096 | -2.11046 | -0.34703 |
| N | 4.239448 | -2.74679 | -0.41012 | C | 4.352832 | -5.79936 | -2.18866 |
| O | 9.180833 | -4.78869 | 0.438725 | C | 5.342521 | -3.88293 | -3.29678 |
| O | -9.18628 | -4.78426 | -0.44027 | C | -6.9898 | -6.23564 | -1.64992 |
| C | -3.23927 | -2.0454 | -0.23656 | C | -5.35282 | -3.87553 | 3.295746 |
| C | -5.17159 | -1.80578 | -1.49046 | C | 9.5686 | -3.59023 | -2.28639 |
| C | -2.3379 | -3.22302 | 1.408705 | C | -10.2873 | -2.10245 | 0.334252 |
| C | 1.181901 | -3.764 | -2.11033 | C | -7.5074 | -7.28017 | -0.62056 |
| C | 3.234015 | -2.04971 | 0.237029 | C | 5.941546 | -6.12879 | -3.99132 |
| C | -5.52992 | -2.79415 | -0.35022 | C | 5.079397 | -6.65554 | -3.02154 |
| C | 2.331447 | -3.22756 | -1.40737 | C | -9.11432 | -2.47444 | 1.285638 |
| C | 1.204018 | -4.05419 | 2.065627 | C | 6.9866 | -6.23618 | 1.657758 |
| C | -1.18905 | -3.76036 | 2.112094 | C | 6.069208 | -4.74158 | -4.12869 |
| C | 5.167466 | -1.80677 | 1.488252 | C | 5.624525 | -6.73167 | 2.199308 |
| C | 3.808565 | -1.4092 | 1.414976 | C | -4.358 | -5.79248 | 2.19311 |
| C | 5.524587 | -2.79835 | 0.350317 | C | -7.9726 | -6.14775 | -2.85238 |
| C | 3.272182 | -0.57319 | 2.39879 | C | -8.7521 | -1.21875 | 2.111176 |
| C | -1.21155 | -4.05443 | -2.06389 | C | -9.58076 | -3.57618 | 2.280334 |
| C | 5.990955 | -1.38405 | 2.522608 | C | -5.6262 | -6.73348 | -2.18537 |
| C | -3.27563 | -0.57434 | -2.4022 | C | 7.973204 | -6.14426 | 2.856797 |
| C | -4.10834 | -0.15187 | -3.44799 | C | 7.500554 | -7.28484 | 0.630921 |
| C | -5.6964 | -4.17092 | -0.948 | C | -5.08521 | -6.64825 | 3.025787 |
| C | -0.06826 | -3.45697 | -1.50177 | C | -6.0799 | -4.73383 | 4.127692 |
| C | 5.692023 | -4.17343 | 0.951853 | C | -5.95007 | -6.12108 | 3.992945 |
| C | 7.896877 | -2.98644 | -0.47395 | H | 6.837316 | 7.343219 | 0.242495 |
| C | 1.123457 | -4.86365 | 3.205665 | H | 8.511325 | 7.021098 | -0.26544 |
| C | -3.69886 | -3.49655 | 1.446078 | H | 7.554754 | 8.267352 | -1.09297 |
| C | -5.99404 | -1.38621 | -2.52695 | H | 8.970682 | 5.846546 | -2.52397 |
| C | 3.692131 | -3.5028 | -1.4443 | H | 7.61174 | 5.425018 | -3.59476 |
| C | 9.105384 | -2.48476 | -1.29438 | H | 8.044613 | 7.12599 | -3.33895 |
| C | -7.90395 | -2.97924 | 0.469719 | H | 5.763615 | 7.723875 | -2.63411 |
| C | 4.106026 | -0.14743 | 3.44235 | H | 5.222341 | 6.07321 | -2.95719 |
| C | -6.85858 | -4.85337 | -0.97535 | H | 4.886065 | 6.833507 | -1.38259 |
| C | 6.854032 | -4.85625 | 0.978575 | H | 7.945635 | 1.410758 | 2.820198 |
| C | 8.053269 | -4.24481 | 0.327865 | H | 8.44996 | 0.374951 | 1.467773 |
| C | -4.486 | -4.39527 | 2.316623 | H | 9.633068 | 0.89379 | 2.675975 |
| C | 5.449265 | -0.54332 | 3.509411 | H | 10.40651 | 3.176625 | 2.889968 |
| C | 4.478555 | -4.40224 | -2.3149 | H | 9.938916 | 4.455075 | 1.750911 |
| C | -0.11022 | -5.10433 | 3.82108 | H | 8.768112 | 3.859593 | 2.949559 |
| C | -1.13189 | -4.86543 | -3.2029 | H | 11.12782 | 1.712991 | 0.91684 |
| C | 0.101553 | -5.1087 | -3.81775 | H | 9.982455 | 1.314749 | -0.37601 |
| C | -5.45144 | -0.54819 | -3.5155 | H | 10.62369 | 2.968991 | -0.23513 |
| C | -8.05919 | -4.23936 | -0.32972 | H | 9.982426 | -1.32064 | 0.352421 |
| C | -1.26784 | -4.55489 | 3.269053 | H | 10.61757 | -2.97815 | 0.221483 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 11.12186 | -1.73251 | -0.9414 | H | -2.22756 | -4.74296 | 3.736715 |
| H | 8.439616 | -0.3912 | -1.48787 | H | 5.221486 | -6.06534 | 2.9713 |
| H | 9.620606 | -0.91536 | -2.69573 | H | 4.879032 | -6.83348 | 1.401789 |
| H | 7.932893 | -1.43323 | -2.83462 | H | 5.759844 | -7.71832 | 2.654959 |
| H | 9.926081 | -4.47337 | -1.75504 | H | 7.613798 | -5.42162 | 3.599771 |
| H | 8.748025 | -3.88619 | -2.95027 | H | 8.045384 | -7.12327 | 3.346125 |
| H | 10.38638 | -3.20225 | -2.90569 | H | 8.968682 | -5.84596 | 2.524839 |
| H | -10.4013 | -3.18634 | 2.894848 | H | 7.543233 | -8.27144 | 1.107906 |
| H | -9.9356 | -4.46171 | 1.751235 | H | 6.822433 | -7.35087 | -0.22833 |
| H | -8.76258 | -3.86874 | 2.948652 | H | 8.49907 | -7.03031 | 0.272183 |
| H | -9.98681 | -1.31466 | -0.36665 | H | -6.5519 | -1.42566 | 1.017411 |
| H | -10.6225 | -2.97149 | -0.23304 | H | -4.79795 | -4.56205 | -1.41014 |
| H | -11.1296 | -1.7225 | 0.925429 | H | -4.79451 | 4.565304 | 1.411929 |
| H | -7.94238 | -1.41758 | 2.822666 | H | -6.54589 | 1.430312 | -1.01953 |
| H | -8.45126 | -0.37957 | 1.473659 | H | 6.550869 | 1.424798 | 1.017541 |
| H | -9.6308 | -0.90239 | 2.683629 | H | 4.798817 | 4.56338 | -1.40853 |
| H | -8.43937 | 0.385334 | -1.47745 | H | 5.451976 | 2.806023 | 3.401151 |
| H | -9.62362 | 0.904039 | -2.68458 | H | 6.753591 | 4.329918 | 4.87081 |
| H | -7.93696 | 1.424015 | -2.82841 | H | 6.514276 | 6.794514 | 4.632615 |
| H | -10.6166 | 2.973073 | 0.230053 | H | 4.960307 | 7.727403 | 2.926493 |
| H | -11.1225 | 1.724466 | -0.92903 | H | 3.663381 | 6.199812 | 1.459655 |
| H | -9.97901 | 1.316596 | 0.36251 | H | 2.226702 | 4.742412 | 3.73939 |
| H | -9.93292 | 4.464326 | -1.75405 | H | 0.169151 | 5.712911 | 4.719976 |
| H | -8.75715 | 3.874948 | -2.9504 | H | -2.03044 | 5.298063 | 3.621794 |
| H | -10.3944 | 3.188866 | -2.89931 | H | -2.1777 | 3.882543 | 1.626555 |
| H | -8.04034 | 7.128598 | 3.340719 | H | 2.235111 | -0.26766 | 2.355356 |
| H | -8.96685 | 5.851756 | 2.522172 | H | 3.693159 | 0.492507 | 4.215112 |
| H | -7.61034 | 5.426583 | 3.59465 | H | 6.072462 | -0.21466 | 4.334903 |
| H | -7.54479 | 8.272444 | 1.09775 | H | 7.024366 | -1.71001 | 2.578614 |
| H | -6.82542 | 7.349686 | -0.23777 | H | 2.237557 | 0.269269 | -2.35634 |
| H | -8.50114 | 7.028986 | 0.265742 | H | 3.693209 | -0.48607 | -4.21981 |
| H | -5.75756 | 7.723798 | 2.640962 | H | 6.072533 | 0.220975 | -4.34052 |
| H | -5.21857 | 6.071954 | 2.961675 | H | 7.026647 | 1.711699 | -2.5815 |
| H | -4.87933 | 6.834423 | 1.388907 | H | -2.18445 | -3.8816 | -1.62302 |
| H | -8.50693 | -7.02378 | -0.26597 | H | -2.03829 | -5.30139 | -3.61518 |
| H | -7.54882 | -8.26865 | -1.09373 | H | 0.161059 | -5.72114 | -4.71195 |
| H | -6.83218 | -7.34307 | 0.241215 | H | 2.219408 | -4.75039 | -3.73334 |
| H | -4.88372 | -6.83388 | -1.38486 | H | 3.675062 | -6.20522 | -1.445 |
| H | -5.76065 | -7.72113 | -2.63913 | H | 4.970288 | -7.73012 | -2.9162 |
| H | -5.21982 | -6.06936 | -2.95751 | H | 6.504111 | -6.7939 | -4.63851 |
| H | -7.61109 | -5.42736 | -3.59651 | H | 6.725443 | -4.32873 | -4.88832 |
| H | -8.04297 | -7.12835 | -3.33884 | H | 5.425782 | -2.8075 | -3.41383 |
| H | -8.96927 | -5.84893 | -2.52452 | H | -5.42842 | 2.804678 | -3.4122 |
| H | 2.177053 | -3.88316 | 1.624336 | H | -3.67219 | 6.204078 | -1.45122 |
| H | 2.029314 | -5.30037 | 3.618334 | H | -4.96689 | 7.727696 | -2.92417 |
| H | -0.17041 | -5.71543 | 4.716144 | H | -6.50316 | 6.79001 | -4.64353 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -6.72746 | 4.324645 | -4.88851 | H | -2.23571 | 0.270599 | 2.357832 |
| H | -2.2185 | 4.74873 | -3.73446 | H | -3.69315 | -0.48478 | 4.220015 |
| H | -0.16003 | 5.720629 | -4.71171 | H | -6.07215 | 0.223412 | 4.339288 |
| H | 2.038677 | 5.303124 | -3.61279 | H | -7.02419 | 1.715589 | 2.580329 |
| H | 2.184147 | 3.884129 | -1.61994 | H | -7.02732 | -1.71255 | -2.58318 |
| H | -3.67815 | -6.19862 | 1.451516 | H | -2.23874 | -0.26835 | -2.35843 |
| H | -4.97447 | -7.72286 | 2.922389 | H | -3.69466 | 0.485774 | -4.22223 |
| H | -6.51302 | -6.78587 | 4.640136 | H | -6.07375 | -0.22202 | -4.34265 |
| H | -6.73821 | -4.3206 | 4.885323 | H | 4.794514 | -4.56273 | 1.417341 |
| H | -5.43772 | -2.80005 | 3.411002 | H | 6.544485 | -1.43351 | -1.02244 |

The Result for the TDDFT calculation

Excited State 1: Singlet-A 1.8052 eV 686.81 nm f=0.0000 <S**2>=0.000
435 -> 439 -0.17972
436 -> 437 0.68098
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -6023.98991014
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.8171 eV 682.32 nm f=0.0000 <S**2>=0.000
435 -> 440 -0.17970
436 -> 438 0.68095

Excited State 3: Singlet-A 1.8487 eV 670.64 nm f=0.0000 <S**2>=0.000
435 -> 437 -0.34810
436 -> 439 0.61138

Excited State 4: Singlet-A 1.8588 eV 667.01 nm f=0.0001 <S**2>=0.000
435 -> 438 -0.33909
436 -> 440 0.61637

Excited State 5: Singlet-A 1.9672 eV 630.25 nm f=0.0002 <S**2>=0.000
435 -> 437 0.61235
436 -> 439 0.35139

Excited State 6: Singlet-A 1.9772 eV 627.06 nm f=0.0000 <S**2>=0.000
435 -> 438 0.61730

436 -> 440 0.34246

Excited State 7: Singlet-A 2.0105 eV 616.68 nm f=0.0000 <S**2>=0.000
435 -> 439 0.68077
436 -> 437 0.18335

Excited State 8: Singlet-A 2.0188 eV 614.15 nm f=0.0002 <S**2>=0.000
435 -> 440 0.68063
436 -> 438 0.18347

Excited State 9: Singlet-A 2.4324 eV 509.73 nm f=0.0015 <S**2>=0.000
429 -> 438 0.10020
432 -> 439 0.11913
433 -> 437 0.12710
434 -> 437 0.66854

Excited State 10: Singlet-A 2.4447 eV 507.16 nm f=0.0000 <S**2>=0.000
429 -> 437 0.11336
432 -> 440 0.13104
433 -> 438 0.14918
434 -> 438 0.65926

Excited State 11: Singlet-A 2.4791 eV 500.13 nm f=0.0003 <S**2>=0.000
429 -> 440 0.13024
432 -> 437 0.30387
433 -> 439 0.22296
434 -> 439 0.55828

Excited State 12: Singlet-A 2.4873 eV 498.47 nm f=0.0001 <S**2>=0.000
429 -> 439 0.14078
431 -> 437 -0.10546
432 -> 438 0.31182
433 -> 440 0.23765
434 -> 440 0.54295

Excited State 13: Singlet-A 2.5031 eV 495.33 nm f=0.0008 <S**2>=0.000

429 -> 438 0.16052
432 -> 439 0.28254
433 -> 437 0.58065
434 -> 437 -0.19515

Excited State 14: Singlet-A 2.5125 eV 493.46 nm f=0.0000 <S**2>=0.000
429 -> 437 0.16694
432 -> 440 0.28022
433 -> 438 0.56816
434 -> 438 -0.22618

Excited State 15: Singlet-A 2.5288 eV 490.29 nm f=0.0001 <S**2>=0.000
432 -> 437 -0.38714
433 -> 439 -0.38520
434 -> 439 0.40972

Excited State 16: Singlet-A 2.5378 eV 488.55 nm f=0.0000 <S**2>=0.000
432 -> 438 -0.37147
433 -> 440 -0.37568
434 -> 440 0.43206

Excited State 17: Singlet-A 2.5966 eV 477.48 nm f=0.0000 <S**2>=0.000
435 -> 443 -0.20187
436 -> 441 0.67153

Excited State 18: Singlet-A 2.6328 eV 470.92 nm f=0.0202 <S**2>=0.000
435 -> 444 -0.24741
436 -> 442 0.65216

Excited State 19: Singlet-A 2.6516 eV 467.59 nm f=0.0058 <S**2>=0.000
435 -> 441 -0.44921
436 -> 443 0.53270

Excited State 20: Singlet-A 2.6592 eV 466.24 nm f=0.0001 <S**2>=0.000
431 -> 438 0.11012
432 -> 437 -0.45073

433 -> 439 0.51111

Excited State 21: Singlet-A 2.6652 eV 465.20 nm f=0.0083 <S**2>=0.000
435 -> 442 -0.39540
436 -> 444 0.56337

Excited State 22: Singlet-A 2.6674 eV 464.80 nm f=0.0006 <S**2>=0.000
431 -> 437 0.14240
432 -> 438 -0.44442
433 -> 440 0.50783

Excited State 23: Singlet-A 2.6733 eV 463.78 nm f=0.0002 <S**2>=0.000
428 -> 440 -0.10049
431 -> 440 -0.14895
432 -> 439 0.58244
433 -> 437 -0.34261

Excited State 24: Singlet-A 2.6805 eV 462.54 nm f=0.0000 <S**2>=0.000
428 -> 439 -0.10331
431 -> 439 -0.16863
432 -> 440 0.57133
433 -> 438 -0.35091

Excited State 25: Singlet-A 2.7282 eV 454.45 nm f=0.0001 <S**2>=0.000
430 -> 438 0.15889
431 -> 437 0.63959
432 -> 438 0.20209

Excited State 26: Singlet-A 2.7377 eV 452.87 nm f=0.0000 <S**2>=0.000
430 -> 437 0.25071
431 -> 438 0.61892
432 -> 437 0.17629

Excited State 27: Singlet-A 2.7757 eV 446.68 nm f=0.0000 <S**2>=0.000
429 -> 437 -0.36184
430 -> 440 0.13698

431 -> 439 0.52288
432 -> 440 0.23717

Excited State 28: Singlet-A 2.7833 eV 445.46 nm f=0.0001 <S**2>=0.000
429 -> 438 -0.35933
430 -> 439 0.18485
431 -> 440 0.52049
432 -> 439 0.21631

Excited State 29: Singlet-A 2.7847 eV 445.24 nm f=0.0000 <S**2>=0.000
430 -> 437 0.64271
431 -> 438 -0.26348

Excited State 30: Singlet-A 2.7957 eV 443.49 nm f=0.0000 <S**2>=0.000
430 -> 438 0.67318
431 -> 437 -0.17788

Excited State 31: Singlet-A 2.8030 eV 442.32 nm f=0.0062 <S**2>=0.000
435 -> 441 0.53844
436 -> 443 0.45434

Excited State 32: Singlet-A 2.8113 eV 441.02 nm f=0.0000 <S**2>=0.000
428 -> 439 -0.20930
429 -> 437 0.52770
430 -> 440 0.14424
431 -> 439 0.35242
433 -> 438 -0.14983

Excited State 33: Singlet-A 2.8192 eV 439.79 nm f=0.0004 <S**2>=0.000
428 -> 440 -0.19949
429 -> 438 0.52489
430 -> 439 0.25147
431 -> 440 0.30293
433 -> 437 -0.14571

Excited State 34: Singlet-A 2.8349 eV 437.35 nm f=0.0000 <S**2>=0.000

428 -> 437 -0.45149
429 -> 439 0.49157
432 -> 438 -0.12424
433 -> 440 -0.17021

Excited State 35: Singlet-A 2.8424 eV 436.20 nm f=0.0016 <S**2>=0.000
428 -> 438 -0.35342
429 -> 440 0.39515
433 -> 439 -0.13030
435 -> 442 -0.35194
436 -> 444 -0.24494

Excited State 36: Singlet-A 2.8432 eV 436.07 nm f=0.0004 <S**2>=0.000
430 -> 439 0.62407
431 -> 440 -0.29543

Excited State 37: Singlet-A 2.8440 eV 435.96 nm f=0.0006 <S**2>=0.000
428 -> 438 -0.27098
429 -> 440 0.30787
435 -> 442 0.45918
436 -> 444 0.31459

Excited State 38: Singlet-A 2.8500 eV 435.03 nm f=0.0000 <S**2>=0.000
430 -> 440 0.66906
431 -> 439 -0.20276

Excited State 39: Singlet-A 2.8592 eV 433.64 nm f=0.0000 <S**2>=0.000
435 -> 443 0.67025
436 -> 441 0.20746

Excited State 40: Singlet-A 2.8743 eV 431.36 nm f=0.0027 <S**2>=0.000
435 -> 444 0.63979
436 -> 442 0.26181

Excited State 41: Singlet-A 2.9206 eV 424.52 nm f=0.0005 <S**2>=0.000
428 -> 437 0.50873

429 -> 439 0.45571

431 -> 437 0.10475

Excited State 42: Singlet-A 2.9297 eV 423.20 nm f=0.0001 <S**2>=0.000

428 -> 438 0.51896

429 -> 440 0.44744

Excited State 43: Singlet-A 2.9477 eV 420.61 nm f=0.0000 <S**2>=0.000

427 -> 437 -0.28883

428 -> 439 0.58613

429 -> 437 0.19677

431 -> 439 0.13124

432 -> 440 0.12287

Excited State 44: Singlet-A 2.9568 eV 419.33 nm f=0.0006 <S**2>=0.000

427 -> 438 -0.26473

428 -> 440 0.59954

429 -> 438 0.20273

431 -> 440 0.11925

432 -> 439 0.11617

Excited State 45: Singlet-A 3.0009 eV 413.15 nm f=0.0000 <S**2>=0.000

427 -> 437 0.62850

428 -> 439 0.29586

Excited State 46: Singlet-A 3.0124 eV 411.58 nm f=0.0002 <S**2>=0.000

427 -> 438 0.64106

428 -> 440 0.27024

Excited State 47: Singlet-A 3.0495 eV 406.57 nm f=0.0000 <S**2>=0.000

413 -> 439 0.18161

414 -> 440 -0.18127

415 -> 437 0.18715

416 -> 438 -0.18896

427 -> 439 0.58344

Excited State 48: Singlet-A 3.0533 eV 406.07 nm f=0.0000 <S**2>=0.000

413 -> 440 -0.30875

414 -> 439 0.30888

415 -> 438 -0.31734

416 -> 437 0.32418

427 -> 440 -0.27513

Excited State 49: Singlet-A 3.0558 eV 405.73 nm f=0.0000 <S**2>=0.000

413 -> 437 0.35594

414 -> 438 -0.35183

415 -> 439 0.33042

416 -> 440 -0.33419

Excited State 50: Singlet-A 3.0559 eV 405.73 nm f=0.0000 <S**2>=0.000

413 -> 438 0.35371

414 -> 437 -0.35335

415 -> 440 0.32854

416 -> 439 -0.33523

Excited State 51: Singlet-A 3.0570 eV 405.58 nm f=0.0000 <S**2>=0.000

413 -> 439 -0.28553

414 -> 440 0.28164

415 -> 437 -0.29365

416 -> 438 0.29671

427 -> 439 0.37491

Excited State 52: Singlet-A 3.0627 eV 404.81 nm f=0.0000 <S**2>=0.000

413 -> 440 -0.13491

414 -> 439 0.13299

415 -> 438 -0.13835

416 -> 437 0.14144

427 -> 440 0.63793

Excited State 53: Singlet-A 3.1610 eV 392.23 nm f=0.0099 <S**2>=0.000

435 -> 446 -0.17677

435 -> 449 0.13249

436 -> 444 -0.13102
436 -> 445 0.60342
436 -> 450 -0.15029
436 -> 457 -0.11693

Excited State 54: Singlet-A 3.1751 eV 390.49 nm f=0.0271 <S**2>=0.000
430 -> 443 -0.11857
433 -> 441 -0.14027
434 -> 441 0.60401
435 -> 445 -0.17040
436 -> 446 0.18445

Excited State 55: Singlet-A 3.1964 eV 387.89 nm f=0.0000 <S**2>=0.000
425 -> 439 -0.17693
426 -> 437 0.68261

Excited State 56: Singlet-A 3.2073 eV 386.56 nm f=0.0000 <S**2>=0.000
425 -> 440 -0.17813
426 -> 438 0.68250

Excited State 57: Singlet-A 3.2342 eV 383.35 nm f=0.1597 <S**2>=0.000
434 -> 441 -0.27963
435 -> 444 0.11279
435 -> 445 -0.37277
436 -> 446 0.44604
436 -> 449 -0.16327

Excited State 58: Singlet-A 3.2397 eV 382.70 nm f=0.0001 <S**2>=0.000
425 -> 437 -0.35471
426 -> 439 0.60954

Excited State 59: Singlet-A 3.2456 eV 382.01 nm f=0.0000 <S**2>=0.000
434 -> 442 0.53694
435 -> 448 0.16355
436 -> 447 -0.34592
436 -> 451 -0.13745

Excited State 60: Singlet-A 3.2488 eV 381.63 nm f=0.0002 <S**2>=0.000

425 -> 438 -0.34642

426 -> 440 0.61398

Excited State 61: Singlet-A 3.2560 eV 380.78 nm f=0.0030 <S**2>=0.000

430 -> 441 -0.21659

433 -> 443 -0.13931

434 -> 443 0.63235

Excited State 62: Singlet-A 3.2685 eV 379.33 nm f=0.0040 <S**2>=0.000

434 -> 444 -0.32222

435 -> 447 -0.21945

435 -> 451 -0.12963

436 -> 448 0.51952

436 -> 452 0.15263

Excited State 63: Singlet-A 3.2996 eV 375.76 nm f=0.0000 <S**2>=0.000

433 -> 442 -0.12676

434 -> 442 0.36590

435 -> 448 -0.14282

436 -> 447 0.55393

Excited State 64: Singlet-A 3.3269 eV 372.67 nm f=0.0004 <S**2>=0.000

431 -> 441 0.15932

433 -> 444 -0.13894

434 -> 444 0.52782

434 -> 445 0.10187

435 -> 447 -0.10186

436 -> 448 0.35488

Excited State 65: Singlet-A 3.3454 eV 370.62 nm f=0.0368 <S**2>=0.000

433 -> 441 0.15553

435 -> 445 0.35467

435 -> 450 -0.15106

436 -> 446 0.48907

436 -> 449 0.21835

Excited State 66: Singlet-A 3.3494 eV 370.17 nm f=0.0000 <S**2>=0.000
425 -> 437 0.61024
426 -> 439 0.35443

Excited State 67: Singlet-A 3.3594 eV 369.07 nm f=0.0001 <S**2>=0.000
425 -> 438 0.61513
426 -> 440 0.34593

Excited State 68: Singlet-A 3.3929 eV 365.42 nm f=0.0001 <S**2>=0.000
425 -> 439 0.68257
426 -> 437 0.17660

Excited State 69: Singlet-A 3.4010 eV 364.55 nm f=0.0000 <S**2>=0.000
425 -> 440 0.68248
426 -> 438 0.17798

Excited State 70: Singlet-A 3.4084 eV 363.76 nm f=0.0086 <S**2>=0.000
432 -> 441 0.30214
433 -> 443 0.14932
435 -> 446 -0.12914
435 -> 449 -0.24702
436 -> 445 0.19551
436 -> 450 0.49033

Excited State 71: Singlet-A 3.4090 eV 363.70 nm f=0.0193 <S**2>=0.000
432 -> 443 0.12170
433 -> 441 0.60797
434 -> 441 0.14967
435 -> 445 -0.21929
436 -> 446 -0.12628

Excited State 72: Singlet-A 3.4195 eV 362.58 nm f=0.0000 <S**2>=0.000
431 -> 443 0.13561
433 -> 442 0.12446

434 -> 442 0.16665
435 -> 448 -0.34759
435 -> 452 -0.24736
436 -> 447 -0.20175
436 -> 451 0.42388

Excited State 73: Singlet-A 3.4213 eV 362.39 nm f=0.0019 <S**2>=0.000
435 -> 446 0.63722
436 -> 445 0.22121
436 -> 450 0.10336

Excited State 74: Singlet-A 3.4321 eV 361.25 nm f=0.0039 <S**2>=0.000
431 -> 441 0.28154
435 -> 447 -0.34531
435 -> 451 -0.22116
436 -> 448 -0.28190
436 -> 452 0.36044

Excited State 75: Singlet-A 3.4390 eV 360.53 nm f=0.0001 <S**2>=0.000
432 -> 442 0.17995
433 -> 444 0.11731
434 -> 444 0.10563
435 -> 447 0.50597
435 -> 451 -0.18610
436 -> 448 0.10323
436 -> 452 0.34969

Excited State 76: Singlet-A 3.4499 eV 359.39 nm f=0.0000 <S**2>=0.000
429 -> 441 0.11497
432 -> 444 0.14766
433 -> 442 0.56969
434 -> 442 0.12903
435 -> 448 0.29797
436 -> 447 0.14326

Excited State 77: Singlet-A 3.4530 eV 359.07 nm f=0.0429 <S**2>=0.000

433 -> 441 -0.20809
435 -> 445 -0.31775
435 -> 450 -0.25293
436 -> 449 0.53128

Excited State 78: Singlet-A 3.4783 eV 356.45 nm f=0.1036 <S**2>=0.000
432 -> 441 0.59127
433 -> 443 0.12537
435 -> 446 0.14558
435 -> 449 0.12128
436 -> 450 -0.28930

Excited State 79: Singlet-A 3.4794 eV 356.34 nm f=0.0000 <S**2>=0.000
433 -> 442 -0.28322
435 -> 448 0.47308
435 -> 452 -0.19924
436 -> 451 0.37168

Excited State 80: Singlet-A 3.4802 eV 356.25 nm f=0.0009 <S**2>=0.000
427 -> 443 0.12120
428 -> 441 -0.14073
431 -> 441 0.55547
433 -> 444 0.10466
434 -> 444 -0.17047
435 -> 447 0.16042
436 -> 452 -0.22724

Excited State 81: Singlet-A 3.5018 eV 354.05 nm f=0.0000 <S**2>=0.000
427 -> 444 0.14179
428 -> 442 -0.10548
430 -> 441 0.17286
431 -> 442 0.55562
433 -> 443 0.31511

Excited State 82: Singlet-A 3.5081 eV 353.43 nm f=0.0763 <S**2>=0.000
432 -> 442 0.56171

433 -> 444 0.30325
434 -> 444 0.11148
435 -> 447 -0.16751
436 -> 452 -0.15290

Excited State 83: Singlet-A 3.5228 eV 351.95 nm f=0.0295 <S**2>=0.000
427 -> 444 -0.11669
428 -> 442 0.14592
430 -> 441 0.38454
431 -> 442 -0.30297
433 -> 443 0.35326
434 -> 443 0.25510

Excited State 84: Singlet-A 3.5529 eV 348.97 nm f=0.0000 <S**2>=0.000
427 -> 441 0.25431
428 -> 443 -0.15866
429 -> 441 -0.11939
430 -> 444 -0.13607
431 -> 443 0.56102
434 -> 442 -0.13415
436 -> 451 -0.11149

Excited State 85: Singlet-A 3.5543 eV 348.83 nm f=0.0006 <S**2>=0.000
428 -> 441 0.12940
429 -> 443 0.14260
430 -> 442 0.20977
432 -> 442 -0.33708
433 -> 444 0.52185
434 -> 444 0.14801

Excited State 86: Singlet-A 3.5562 eV 348.64 nm f=0.0887 <S**2>=0.000
427 -> 442 0.24619
428 -> 444 -0.17519
430 -> 443 -0.14759
431 -> 444 0.57489
431 -> 445 0.10299

Excited State 87: Singlet-A 3.5655 eV 347.74 nm f=0.0217 <S**2>=0.000

430 -> 441 0.50224

432 -> 441 0.13459

433 -> 443 -0.44535

Excited State 88: Singlet-A 3.5691 eV 347.38 nm f=0.0247 <S**2>=0.000

429 -> 442 -0.10938

431 -> 444 -0.11456

432 -> 443 0.67042

433 -> 441 -0.10225

Excited State 89: Singlet-A 3.5927 eV 345.10 nm f=0.0000 <S**2>=0.000

429 -> 441 -0.19593

431 -> 443 -0.13040

432 -> 444 0.64477

433 -> 442 -0.11494

Excited State 90: Singlet-A 3.6055 eV 343.88 nm f=0.0000 <S**2>=0.000

424 -> 437 0.70380

Excited State 91: Singlet-A 3.6173 eV 342.76 nm f=0.0001 <S**2>=0.000

424 -> 438 0.70465

Excited State 92: Singlet-A 3.6245 eV 342.07 nm f=0.0001 <S**2>=0.000

435 -> 445 0.10317

435 -> 450 0.55026

435 -> 457 0.14458

435 -> 460 -0.13607

436 -> 449 0.33181

Excited State 93: Singlet-A 3.6250 eV 342.03 nm f=0.0050 <S**2>=0.000

435 -> 449 0.56634

436 -> 450 0.21243

436 -> 457 0.19841

436 -> 460 -0.20180

436 -> 465 -0.12256

Excited State 94: Singlet-A 3.6300 eV 341.55 nm f=0.0040 <S**2>=0.000
430 -> 442 0.62600
433 -> 444 -0.24081
436 -> 452 -0.11729

Excited State 95: Singlet-A 3.6410 eV 340.53 nm f=0.1542 <S**2>=0.000
430 -> 443 0.63832
431 -> 444 0.15598
433 -> 441 -0.10510

Excited State 96: Singlet-A 3.6605 eV 338.71 nm f=0.0000 <S**2>=0.000
428 -> 443 -0.22518
429 -> 441 0.60344
432 -> 444 0.13561
433 -> 442 -0.16027
436 -> 451 -0.10953

Excited State 97: Singlet-A 3.6648 eV 338.31 nm f=0.0006 <S**2>=0.000
424 -> 439 0.70417

Excited State 98: Singlet-A 3.6671 eV 338.10 nm f=0.0000 <S**2>=0.000
429 -> 441 -0.15250
430 -> 444 0.50887
430 -> 445 0.11184
431 -> 443 0.10067
435 -> 452 -0.27665
436 -> 451 -0.25388

Excited State 99: Singlet-A 3.6735 eV 337.51 nm f=0.0000 <S**2>=0.000
424 -> 440 0.70367

Excited State 100: Singlet-A 3.6841 eV 336.54 nm f=0.0032 <S**2>=0.000
430 -> 442 0.10839
435 -> 451 0.58142

436 -> 452 0.33390

Excited State 101: Singlet-A 3.6847 eV 336.49 nm f=0.0191 <S**2>=0.000
435 -> 449 0.24674
435 -> 468 -0.12037
436 -> 445 -0.14303
436 -> 450 0.28636
436 -> 453 0.10687
436 -> 457 -0.31536
436 -> 460 0.32567
436 -> 465 0.20919

Excited State 102: Singlet-A 3.6909 eV 335.92 nm f=0.0000 <S**2>=0.000
430 -> 444 0.33412
431 -> 443 0.13467
435 -> 452 0.52883
436 -> 451 0.22937

Excited State 103: Singlet-A 3.7020 eV 334.92 nm f=0.0135 <S**2>=0.000
428 -> 444 -0.22924
429 -> 442 0.64406

Excited State 104: Singlet-A 3.7030 eV 334.82 nm f=0.0541 <S**2>=0.000
428 -> 441 0.57010
429 -> 443 -0.33709
431 -> 441 0.14577
435 -> 451 -0.10535

Excited State 105: Singlet-A 3.7414 eV 331.39 nm f=0.0910 <S**2>=0.000
428 -> 442 0.53983
429 -> 444 -0.39752
431 -> 442 0.13899

Excited State 106: Singlet-A 3.7610 eV 329.65 nm f=0.0007 <S**2>=0.000
434 -> 444 -0.15192
434 -> 445 0.59232

434 -> 450 -0.15321
434 -> 457 -0.15660
434 -> 460 0.10196

Excited State 107: Singlet-A 3.7681 eV 329.04 nm f=0.0000 <S**2>=0.000
427 -> 441 0.58883
428 -> 443 -0.11230
430 -> 444 0.13116
431 -> 443 -0.29294
432 -> 444 -0.10253

Excited State 108: Singlet-A 3.7704 eV 328.84 nm f=0.0272 <S**2>=0.000
435 -> 445 -0.15623
435 -> 450 0.26563
435 -> 453 0.13864
435 -> 457 -0.30771
435 -> 460 0.32021
435 -> 465 0.20728
436 -> 454 0.17440
436 -> 468 -0.16257
436 -> 470 -0.13187

Excited State 109: Singlet-A 3.7916 eV 327.00 nm f=0.0000 <S**2>=0.000
418 -> 438 -0.12252
420 -> 439 -0.11502
422 -> 440 -0.11366
423 -> 437 0.66915

Excited State 110: Singlet-A 3.7958 eV 326.63 nm f=0.0118 <S**2>=0.000
427 -> 443 -0.22122
428 -> 441 0.24679
429 -> 443 0.55903
431 -> 441 0.14371
432 -> 442 0.12198
433 -> 444 -0.12074

Excited State 111: Singlet-A 3.8012 eV 326.17 nm f=0.0007 <S**2>=0.000

418 -> 437 -0.13458

420 -> 440 -0.12117

422 -> 439 -0.13035

423 -> 438 0.66078

Excited State 112: Singlet-A 3.8086 eV 325.54 nm f=0.0257 <S**2>=0.000

427 -> 442 0.58520

428 -> 444 -0.17191

431 -> 444 -0.29005

Excited State 113: Singlet-A 3.8164 eV 324.87 nm f=0.0040 <S**2>=0.000

427 -> 444 -0.34574

428 -> 442 0.24264

429 -> 444 0.48174

431 -> 442 0.21139

Excited State 114: Singlet-A 3.8339 eV 323.39 nm f=0.0000 <S**2>=0.000

418 -> 440 -0.14362

420 -> 437 -0.24447

422 -> 438 -0.31028

423 -> 439 0.54836

Excited State 115: Singlet-A 3.8370 eV 323.13 nm f=0.0036 <S**2>=0.000

418 -> 439 -0.15125

420 -> 438 -0.24694

422 -> 437 -0.35979

423 -> 440 0.50182

Excited State 116: Singlet-A 3.8434 eV 322.59 nm f=0.0022 <S**2>=0.000

434 -> 448 0.11933

435 -> 454 0.27851

436 -> 453 0.59042

436 -> 457 0.12605

Excited State 117: Singlet-A 3.8486 eV 322.16 nm f=0.0000 <S**2>=0.000

427 -> 441 0.20535
428 -> 443 0.61374
429 -> 441 0.17093
432 -> 444 0.13136

Excited State 118: Singlet-A 3.8521 eV 321.86 nm f=0.0077 <S**2>=0.000
435 -> 453 0.26677
435 -> 457 0.15046
435 -> 460 -0.10984
436 -> 454 0.57034

Excited State 119: Singlet-A 3.8554 eV 321.58 nm f=0.0004 <S**2>=0.000
427 -> 443 0.60916
428 -> 441 0.21899
429 -> 443 0.18568

Excited State 120: Singlet-A 3.8633 eV 320.93 nm f=0.0000 <S**2>=0.000
430 -> 444 0.15353
430 -> 445 -0.17632
434 -> 446 0.60469
434 -> 449 -0.18086

Excited State 121: Singlet-A 3.8689 eV 320.47 nm f=0.0008 <S**2>=0.000
435 -> 456 -0.28494
436 -> 455 0.62158

Excited State 122: Singlet-A 3.8710 eV 320.29 nm f=0.0002 <S**2>=0.000
427 -> 444 0.49840
427 -> 445 0.11106
428 -> 442 0.29033
429 -> 444 0.26964
434 -> 448 0.19027

Excited State 123: Singlet-A 3.8727 eV 320.15 nm f=0.0000 <S**2>=0.000
435 -> 455 -0.29858
436 -> 456 0.61704

Excited State 124: Singlet-A 3.8733 eV 320.10 nm f=0.0014 <S**2>=0.000

427 -> 444 -0.17976

428 -> 442 -0.10334

430 -> 447 -0.10732

430 -> 451 -0.10173

434 -> 448 0.56360

434 -> 452 0.17342

436 -> 453 -0.13427

Excited State 125: Singlet-A 3.8746 eV 319.99 nm f=0.0002 <S**2>=0.000

427 -> 442 -0.13818

428 -> 444 -0.34966

429 -> 442 -0.11843

430 -> 443 -0.10846

434 -> 447 0.49649

434 -> 451 0.14472

Excited State 126: Singlet-A 3.8834 eV 319.27 nm f=0.0068 <S**2>=0.000

427 -> 442 0.23341

428 -> 444 0.47402

429 -> 442 0.14380

434 -> 447 0.35631

434 -> 451 0.10441

Excited State 127: Singlet-A 3.9049 eV 317.51 nm f=0.0012 <S**2>=0.000

420 -> 438 0.18582

422 -> 437 0.48378

423 -> 440 0.46323

Excited State 128: Singlet-A 3.9058 eV 317.44 nm f=0.0000 <S**2>=0.000

420 -> 437 0.23777

422 -> 438 0.49390

423 -> 439 0.42022

Excited State 129: Singlet-A 3.9289 eV 315.57 nm f=0.0016 <S**2>=0.000

417 -> 437 -0.10283
417 -> 438 -0.12168
418 -> 437 0.15623
418 -> 438 0.12487
420 -> 439 0.17907
420 -> 440 0.21251
421 -> 437 -0.16306
421 -> 438 -0.15377
422 -> 439 0.39518
422 -> 440 0.29117
423 -> 437 0.12726
423 -> 438 0.17450

Excited State 130: Singlet-A 3.9290 eV 315.56 nm f=0.0013 <S**2>=0.000
417 -> 437 -0.12800
418 -> 437 -0.12434
418 -> 438 0.15728
420 -> 439 0.22225
420 -> 440 -0.17157
421 -> 437 -0.20343
421 -> 438 0.12376
422 -> 439 -0.31294
422 -> 440 0.36776
423 -> 437 0.15826
423 -> 438 -0.14005

Excited State 131: Singlet-A 3.9661 eV 312.61 nm f=0.0061 <S**2>=0.000
429 -> 448 -0.11801
432 -> 446 0.23275
433 -> 445 0.58131
436 -> 455 -0.12672

Excited State 132: Singlet-A 3.9713 eV 312.20 nm f=0.0038 <S**2>=0.000
420 -> 439 0.11528
421 -> 437 0.64127
422 -> 440 0.23070

Excited State 133: Singlet-A 3.9809 eV 311.45 nm f=0.0001 <S**2>=0.000

421 -> 438 0.65851

422 -> 439 0.21004

Excited State 134: Singlet-A 3.9899 eV 310.75 nm f=0.0000 <S**2>=0.000

426 -> 442 0.10259

429 -> 447 -0.10638

432 -> 445 0.41386

433 -> 446 0.44414

436 -> 456 -0.13370

Excited State 135: Singlet-A 3.9991 eV 310.03 nm f=0.0237 <S**2>=0.000

425 -> 443 -0.14468

426 -> 441 0.45574

431 -> 445 -0.10196

432 -> 448 -0.16961

433 -> 447 -0.32525

435 -> 453 0.16677

436 -> 454 -0.16253

Excited State 136: Singlet-A 4.0076 eV 309.37 nm f=0.0071 <S**2>=0.000

426 -> 441 0.22488

430 -> 452 -0.12713

431 -> 445 0.28292

434 -> 447 -0.23170

434 -> 451 0.34345

436 -> 454 0.10781

436 -> 458 -0.11003

436 -> 462 0.10615

Excited State 137: Singlet-A 4.0081 eV 309.33 nm f=0.0000 <S**2>=0.000

408 -> 438 -0.13550

409 -> 440 -0.13660

410 -> 437 -0.17302

411 -> 439 0.13952

412 -> 438 0.11104
430 -> 444 -0.10890
430 -> 445 0.22481
430 -> 450 -0.13296
434 -> 446 0.26676
434 -> 449 0.38895

Excited State 138: Singlet-A 4.0117 eV 309.06 nm f=0.0005 <S**2>=0.000
408 -> 437 0.23147
409 -> 439 0.24900
410 -> 438 0.31025
411 -> 440 -0.24048
412 -> 437 -0.22834
419 -> 438 -0.13184
421 -> 440 -0.11000
426 -> 441 0.20882
436 -> 458 0.10703

Excited State 139: Singlet-A 4.0125 eV 308.99 nm f=0.0097 <S**2>=0.000
403 -> 437 -0.10409
404 -> 438 0.11919
408 -> 439 0.17849
409 -> 437 0.28775
410 -> 440 0.24247
411 -> 438 -0.27750
412 -> 439 -0.17214
415 -> 438 0.10237
432 -> 447 0.10746
433 -> 448 0.19981
435 -> 454 0.15441
436 -> 453 -0.12264

Excited State 140: Singlet-A 4.0128 eV 308.97 nm f=0.0003 <S**2>=0.000
408 -> 438 0.17436
409 -> 440 0.20556
410 -> 437 0.26874

411 -> 439 -0.20099
412 -> 438 -0.20934
419 -> 437 -0.11648
421 -> 439 -0.20271
430 -> 445 0.12386
433 -> 446 0.13708
434 -> 446 0.14028
434 -> 449 0.20580

Excited State 141: Singlet-A 4.0133 eV 308.93 nm f=0.0006 <S**2>=0.000
403 -> 438 0.11661
404 -> 437 -0.13961
408 -> 440 -0.20500
409 -> 438 -0.32503
410 -> 439 -0.28695
411 -> 437 0.32800
412 -> 440 0.19528
415 -> 437 -0.12210
416 -> 438 0.10147

Excited State 142: Singlet-A 4.0160 eV 308.72 nm f=0.0064 <S**2>=0.000
408 -> 439 -0.10184
409 -> 437 -0.15461
410 -> 440 -0.13484
411 -> 438 0.14933
429 -> 445 -0.12507
432 -> 447 0.19244
433 -> 448 0.36239
435 -> 454 0.30848
435 -> 458 0.10703
436 -> 453 -0.22038

Excited State 143: Singlet-A 4.0181 eV 308.56 nm f=0.0000 <S**2>=0.000
421 -> 440 -0.10954
426 -> 441 -0.27118
433 -> 447 -0.18373

434 -> 451 0.11161
435 -> 453 0.44837
436 -> 454 -0.21374
436 -> 458 -0.20126

Excited State 144: Singlet-A 4.0248 eV 308.05 nm f=0.0000 <S**2>=0.000
408 -> 438 0.11846
410 -> 437 0.12631
411 -> 439 -0.10451
420 -> 437 -0.12276
421 -> 439 0.59482
422 -> 438 0.18917

Excited State 145: Singlet-A 4.0306 eV 307.60 nm f=0.0038 <S**2>=0.000
418 -> 439 -0.10911
420 -> 438 -0.23067
421 -> 440 0.52918
422 -> 437 0.22763

Excited State 146: Singlet-A 4.0359 eV 307.20 nm f=0.0000 <S**2>=0.000
420 -> 437 -0.14975
422 -> 438 0.10108
432 -> 445 0.12357
435 -> 455 0.49414
436 -> 456 0.19184
436 -> 459 0.35373

Excited State 147: Singlet-A 4.0363 eV 307.17 nm f=0.0094 <S**2>=0.000
430 -> 451 -0.12419
432 -> 447 -0.13398
433 -> 448 -0.19385
434 -> 448 -0.22624
434 -> 452 0.37234
435 -> 454 0.20809
435 -> 458 0.15868
436 -> 453 -0.11704

436 -> 457 0.18568
436 -> 460 0.12735
436 -> 465 0.11489

Excited State 148: Singlet-A 4.0380 eV 307.04 nm f=0.0000 <S**2>=0.000
417 -> 439 -0.17614
420 -> 437 0.46236
421 -> 439 0.25953
422 -> 438 -0.30129
435 -> 455 0.16303
436 -> 459 0.10942

Excited State 149: Singlet-A 4.0405 eV 306.85 nm f=0.0098 <S**2>=0.000
426 -> 441 0.23701
431 -> 445 0.15839
432 -> 448 0.20038
433 -> 447 0.35303
434 -> 447 0.10637
434 -> 451 -0.20444
435 -> 453 0.30716
436 -> 458 -0.15793

Excited State 150: Singlet-A 4.0437 eV 306.61 nm f=0.0061 <S**2>=0.000
425 -> 441 -0.12518
426 -> 443 0.13676
432 -> 447 -0.19572
433 -> 448 -0.18942
434 -> 448 0.11508
434 -> 450 0.13033
434 -> 452 -0.18289
435 -> 454 0.45609
436 -> 453 -0.13398
436 -> 457 -0.12980
436 -> 460 -0.12875

Excited State 151: Singlet-A 4.0438 eV 306.60 nm f=0.0071 <S**2>=0.000

417 -> 440 -0.10798
420 -> 438 0.27454
421 -> 440 0.24432
422 -> 437 -0.14820
434 -> 445 0.19645
434 -> 450 0.41405

Excited State 152: Singlet-A 4.0438 eV 306.60 nm f=0.0043 <S**2>=0.000
417 -> 440 -0.13974
420 -> 438 0.35544
421 -> 440 0.31805
422 -> 437 -0.19163
434 -> 445 -0.15285
434 -> 450 -0.32225

Excited State 153: Singlet-A 4.0530 eV 305.91 nm f=0.0008 <S**2>=0.000
428 -> 445 -0.10424
430 -> 452 0.11297
431 -> 445 0.35337
431 -> 450 -0.11668
431 -> 457 -0.10114
432 -> 448 -0.12498
433 -> 447 -0.30241
434 -> 447 0.10693
434 -> 451 -0.31925
435 -> 453 -0.11235

Excited State 154: Singlet-A 4.0536 eV 305.86 nm f=0.0007 <S**2>=0.000
417 -> 437 -0.12439
422 -> 440 -0.12489
432 -> 446 0.11529
435 -> 456 0.57216
435 -> 459 0.12688
436 -> 455 0.25011

Excited State 155: Singlet-A 4.0561 eV 305.67 nm f=0.0008 <S**2>=0.000

401 -> 438 -0.11503
403 -> 437 -0.15225
417 -> 438 0.35336
418 -> 437 -0.29373
419 -> 440 0.11022
420 -> 440 -0.16119
422 -> 439 0.35584
436 -> 457 0.10192

Excited State 156: Singlet-A 4.0571 eV 305.60 nm f=0.0003 <S**2>=0.000
401 -> 437 -0.10602
403 -> 438 -0.13789
417 -> 437 0.34477
418 -> 438 -0.24236
419 -> 439 0.11757
420 -> 439 -0.15099
422 -> 440 0.35810
434 -> 450 0.12541
435 -> 456 0.21202

Excited State 157: Singlet-A 4.0601 eV 305.38 nm f=0.0111 <S**2>=0.000
431 -> 445 0.27205
432 -> 452 -0.12163
433 -> 451 -0.14766
435 -> 457 0.19087
435 -> 460 0.14351
436 -> 458 0.44140
436 -> 462 -0.19362

Excited State 158: Singlet-A 4.0642 eV 305.06 nm f=0.0000 <S**2>=0.000
425 -> 441 -0.18881
426 -> 443 0.19681
430 -> 451 -0.11230
432 -> 447 0.19188
433 -> 448 0.15493
433 -> 452 -0.15024

434 -> 448 -0.15428
434 -> 452 0.29533
435 -> 458 -0.17941
435 -> 462 0.10035
436 -> 457 -0.27046
436 -> 460 -0.19351
436 -> 465 -0.11787

Excited State 159: Singlet-A 4.0646 eV 305.03 nm f=0.0000 <S**2>=0.000
419 -> 437 -0.11292
425 -> 444 -0.19312
426 -> 442 0.61120
432 -> 445 -0.12245

Excited State 160: Singlet-A 4.0739 eV 304.34 nm f=0.0134 <S**2>=0.000
404 -> 438 0.14356
406 -> 437 -0.15300
407 -> 440 0.12463
408 -> 439 -0.10475
425 -> 441 0.37290
426 -> 443 -0.36479
433 -> 448 -0.11419
434 -> 452 0.10750
436 -> 457 -0.15962
436 -> 460 -0.12288

Excited State 161: Singlet-A 4.0760 eV 304.18 nm f=0.0000 <S**2>=0.000
400 -> 437 0.10755
402 -> 438 0.10405
404 -> 439 0.22043
405 -> 438 0.15292
406 -> 440 -0.21263
407 -> 437 0.23117
408 -> 438 -0.16342
412 -> 438 -0.11189
419 -> 437 0.39547

420 -> 437 0.12799
426 -> 442 0.19866

Excited State 162: Singlet-A 4.0790 eV 303.96 nm f=0.0175 <S**2>=0.000
400 -> 438 0.10707
402 -> 437 0.11200
404 -> 440 0.24338
405 -> 437 0.18207
406 -> 439 -0.24648
407 -> 438 0.26696
408 -> 437 -0.20207
411 -> 440 0.10410
412 -> 437 -0.12539
419 -> 438 0.35403
420 -> 438 0.11444

Excited State 163: Singlet-A 4.0803 eV 303.86 nm f=0.0000 <S**2>=0.000
429 -> 447 -0.10728
432 -> 445 -0.21044
432 -> 450 0.16585
433 -> 446 0.35740
433 -> 449 0.22958
435 -> 455 0.12312
435 -> 461 -0.14100
435 -> 464 0.18062
436 -> 463 0.32910

Excited State 164: Singlet-A 4.0807 eV 303.83 nm f=0.0009 <S**2>=0.000
404 -> 437 -0.29350
405 -> 440 -0.14872
406 -> 438 0.29499
407 -> 439 -0.24298
408 -> 440 0.18715
409 -> 438 0.10658
411 -> 437 -0.15059
412 -> 440 0.10103

419 -> 439 -0.16759
432 -> 446 -0.14745
433 -> 450 -0.10966

Excited State 165: Singlet-A 4.0849 eV 303.52 nm f=0.0432 <S**2>=0.000
404 -> 438 -0.27543
405 -> 439 -0.14194
406 -> 437 0.28974
407 -> 440 -0.22710
408 -> 439 0.18572
409 -> 437 0.10730
411 -> 438 -0.14172
418 -> 437 -0.10450
419 -> 440 -0.14961
425 -> 441 0.19752
426 -> 443 -0.18199
434 -> 452 0.10786

Excited State 166: Singlet-A 4.0882 eV 303.28 nm f=0.0071 <S**2>=0.000
404 -> 437 0.11023
406 -> 438 -0.11124
432 -> 446 -0.21742
432 -> 449 -0.17433
433 -> 450 -0.22142
435 -> 463 0.24409
436 -> 461 -0.30737
436 -> 464 0.31202

Excited State 167: Singlet-A 4.0959 eV 302.70 nm f=0.0000 <S**2>=0.000
432 -> 445 -0.29383
433 -> 446 0.19228
434 -> 449 -0.12515
435 -> 455 -0.19683
435 -> 461 0.17588
436 -> 456 -0.14145
436 -> 459 0.46936

Excited State 168: Singlet-A 4.1038 eV 302.12 nm f=0.0032 <S**2>=0.000

425 -> 442 -0.31081
426 -> 444 0.35497
431 -> 447 0.12464
432 -> 446 0.32688
433 -> 445 -0.25942
436 -> 461 -0.15147

Excited State 169: Singlet-A 4.1073 eV 301.87 nm f=0.0000 <S**2>=0.000

400 -> 437 -0.10357
401 -> 439 0.11440
403 -> 440 0.11730
404 -> 439 0.10226
405 -> 438 0.17775
406 -> 440 -0.12277
407 -> 437 0.25550
408 -> 438 -0.13733
417 -> 439 -0.24295
418 -> 440 0.25192
419 -> 437 -0.24993
420 -> 437 -0.25274

Excited State 170: Singlet-A 4.1099 eV 301.67 nm f=0.0000 <S**2>=0.000

430 -> 445 -0.16609
431 -> 448 0.18189
432 -> 445 0.22029
432 -> 450 0.15213
433 -> 446 -0.20910
433 -> 449 0.12620
434 -> 449 0.22613
435 -> 455 -0.23817
435 -> 464 0.14014
436 -> 456 -0.13000
436 -> 459 0.25457
436 -> 463 0.23526

Excited State 171: Singlet-A 4.1100 eV 301.66 nm f=0.0152 <S**2>=0.000

400 -> 438 0.11766
401 -> 440 -0.12414
403 -> 439 -0.13302
405 -> 437 -0.16444
407 -> 438 -0.21595
408 -> 437 0.10870
416 -> 439 -0.10756
417 -> 440 0.24289
418 -> 439 -0.27837
419 -> 438 0.24100
420 -> 438 0.29306

Excited State 172: Singlet-A 4.1174 eV 301.12 nm f=0.0171 <S**2>=0.000

418 -> 438 -0.29005
420 -> 439 0.40396
422 -> 440 -0.11809
425 -> 442 0.23559
426 -> 444 -0.27592
432 -> 446 0.22996

Excited State 173: Singlet-A 4.1176 eV 301.11 nm f=0.0035 <S**2>=0.000

418 -> 437 -0.29854
420 -> 440 0.40867
422 -> 439 -0.11389
431 -> 446 -0.18860
432 -> 447 -0.29126
433 -> 448 0.23141
434 -> 452 0.12168

Excited State 174: Singlet-A 4.1193 eV 300.98 nm f=0.0243 <S**2>=0.000

418 -> 438 -0.18689
420 -> 439 0.38000
422 -> 440 -0.11052
425 -> 442 -0.21536

426 -> 444 0.24569
431 -> 447 -0.12042
432 -> 446 -0.30234
433 -> 445 0.12393
436 -> 461 0.12500

Excited State 175: Singlet-A 4.1232 eV 300.70 nm f=0.0014 <S**2>=0.000
418 -> 437 -0.23411
420 -> 440 0.37800
427 -> 445 0.10735
431 -> 446 0.28856
432 -> 447 0.28123
433 -> 448 -0.25906

Excited State 176: Singlet-A 4.1322 eV 300.04 nm f=0.0130 <S**2>=0.000
419 -> 438 0.13311
428 -> 445 0.14663
432 -> 448 0.56062
433 -> 447 -0.28500

Excited State 177: Singlet-A 4.1324 eV 300.03 nm f=0.0005 <S**2>=0.000
417 -> 439 -0.12917
418 -> 440 0.14020
419 -> 437 0.25685
420 -> 437 -0.11604
430 -> 445 0.16612
431 -> 448 -0.19779
431 -> 452 -0.10133
432 -> 445 0.21314
432 -> 448 -0.11503
434 -> 449 -0.22014
436 -> 463 0.17016

Excited State 178: Singlet-A 4.1360 eV 299.77 nm f=0.0000 <S**2>=0.000
408 -> 438 0.10436
410 -> 437 0.10830

417 -> 439 -0.12830
418 -> 440 0.15402
419 -> 437 0.37763
430 -> 445 -0.18062
431 -> 448 0.17867
432 -> 445 -0.12708
434 -> 449 0.21815
436 -> 463 -0.11172

Excited State 179: Singlet-A 4.1402 eV 299.47 nm f=0.0016 <S**2>=0.000
401 -> 438 0.10335
403 -> 437 0.10527
420 -> 440 -0.10568
427 -> 444 -0.12302
427 -> 445 0.19784
428 -> 446 -0.11898
429 -> 445 -0.15616
431 -> 446 0.34765
431 -> 449 -0.17128
432 -> 447 -0.31117

Excited State 180: Singlet-A 4.1404 eV 299.45 nm f=0.0105 <S**2>=0.000
406 -> 439 0.10213
408 -> 437 0.11026
410 -> 438 0.11549
417 -> 440 -0.12729
418 -> 439 0.17994
419 -> 438 0.43792
433 -> 451 -0.10705
435 -> 465 0.10057
436 -> 458 -0.17821
436 -> 462 -0.20899

Excited State 181: Singlet-A 4.1412 eV 299.39 nm f=0.0001 <S**2>=0.000
433 -> 450 -0.12679
435 -> 456 -0.10950

435 -> 459 0.36021
435 -> 463 0.12125
436 -> 461 0.36359
436 -> 464 0.28496
436 -> 467 0.11074

Excited State 182: Singlet-A 4.1424 eV 299.30 nm f=0.0106 <S**2>=0.000
400 -> 440 0.11431
401 -> 438 -0.20193
403 -> 437 -0.20807
404 -> 438 -0.12240
405 -> 439 -0.16862
406 -> 437 0.17259
407 -> 440 -0.12778
413 -> 440 -0.12983
414 -> 439 0.13653
415 -> 438 0.15108
416 -> 437 -0.17823
418 -> 437 0.25768
431 -> 446 0.13130
432 -> 447 -0.19707

Excited State 183: Singlet-A 4.1430 eV 299.26 nm f=0.0113 <S**2>=0.000
418 -> 439 0.10408
419 -> 438 0.24749
432 -> 452 0.14529
433 -> 451 0.17867
435 -> 453 0.16032
435 -> 465 -0.17152
436 -> 458 0.29896
436 -> 462 0.39340

Excited State 184: Singlet-A 4.1447 eV 299.14 nm f=0.0003 <S**2>=0.000
400 -> 439 0.11509
401 -> 437 -0.20516
403 -> 438 -0.19936

404 -> 437 -0.12806
405 -> 440 -0.15911
406 -> 438 0.17062
407 -> 439 -0.12224
413 -> 439 -0.13818
414 -> 440 0.13991
415 -> 437 0.17072
416 -> 438 -0.17700
418 -> 438 0.30241
419 -> 439 0.13165
432 -> 446 0.10261
435 -> 459 0.12670
436 -> 461 0.11932

Excited State 185: Singlet-A 4.1563 eV 298.31 nm f=0.0016 <S**2>=0.000
419 -> 439 -0.12158
427 -> 443 0.10636
427 -> 448 0.12960
428 -> 447 -0.10971
429 -> 448 -0.11033
431 -> 447 0.44403
431 -> 451 0.16250
432 -> 446 -0.20256
434 -> 450 0.18744
434 -> 460 0.10867

Excited State 186: Singlet-A 4.1641 eV 297.75 nm f=0.0022 <S**2>=0.000
399 -> 437 -0.10917
400 -> 438 0.13903
401 -> 440 -0.13817
403 -> 439 -0.13313
405 -> 437 -0.18163
406 -> 439 0.11357
409 -> 439 -0.10143
413 -> 438 -0.16957
414 -> 437 0.15698

415 -> 440 0.20588
416 -> 439 -0.20662
417 -> 440 -0.10766
418 -> 439 0.40642

Excited State 187: Singlet-A 4.1666 eV 297.57 nm f=0.0000 <S**2>=0.000
399 -> 438 -0.10136
400 -> 437 0.13401
401 -> 439 -0.13323
403 -> 440 -0.11967
405 -> 438 -0.16970
406 -> 440 0.11461
413 -> 437 -0.18305
414 -> 438 0.15851
415 -> 439 0.22402
416 -> 440 -0.20830
417 -> 439 -0.14216
418 -> 440 0.40088

Excited State 188: Singlet-A 4.1738 eV 297.05 nm f=0.0014 <S**2>=0.000
419 -> 440 -0.23423
429 -> 450 0.11719
432 -> 451 0.26904
433 -> 452 0.33727
435 -> 458 -0.16986
435 -> 462 -0.20304
436 -> 457 -0.14742
436 -> 460 -0.22902
436 -> 465 0.20564

Excited State 189: Singlet-A 4.1744 eV 297.01 nm f=0.0001 <S**2>=0.000
410 -> 439 0.11412
413 -> 439 0.10055
419 -> 439 0.61248
431 -> 447 0.12491

Excited State 190: Singlet-A 4.1831 eV 296.39 nm f=0.0004 <S**2>=0.000

410 -> 440 0.10320

419 -> 440 0.59613

432 -> 451 0.10514

433 -> 452 0.13324

436 -> 460 -0.10017

Excited State 191: Singlet-A 4.1898 eV 295.92 nm f=0.0000 <S**2>=0.000

430 -> 445 0.39055

431 -> 448 0.46274

431 -> 452 0.11902

434 -> 449 -0.19184

Excited State 192: Singlet-A 4.1937 eV 295.64 nm f=0.0226 <S**2>=0.000

429 -> 448 -0.10969

430 -> 446 -0.27266

430 -> 449 0.10544

432 -> 449 0.24279

433 -> 450 0.36315

434 -> 460 -0.11383

434 -> 465 -0.10052

436 -> 461 -0.10211

436 -> 464 0.23222

Excited State 193: Singlet-A 4.2023 eV 295.04 nm f=0.0042 <S**2>=0.000

403 -> 438 -0.11611

413 -> 439 0.22233

414 -> 440 -0.23287

415 -> 437 -0.25775

416 -> 438 0.18872

417 -> 437 0.34542

418 -> 438 0.28118

420 -> 439 0.11329

Excited State 194: Singlet-A 4.2032 eV 294.98 nm f=0.0000 <S**2>=0.000

401 -> 438 -0.10051

403 -> 437 -0.14484
413 -> 440 0.24307
414 -> 439 -0.26858
415 -> 438 -0.26460
416 -> 437 0.22612
417 -> 438 0.31819
418 -> 437 0.22511
419 -> 440 -0.11172
420 -> 440 0.12630

Excited State 195: Singlet-A 4.2043 eV 294.90 nm f=0.0155 <S**2>=0.000
399 -> 437 0.17126
400 -> 438 -0.23378
401 -> 440 0.13697
402 -> 437 -0.15321
403 -> 439 0.15420
405 -> 437 0.13625
412 -> 437 0.10071
413 -> 438 -0.23763
414 -> 437 0.28795
415 -> 440 0.25933
416 -> 439 -0.25162
418 -> 439 -0.11445

Excited State 196: Singlet-A 4.2056 eV 294.81 nm f=0.0000 <S**2>=0.000
399 -> 438 0.17386
400 -> 437 -0.24779
401 -> 439 0.14529
402 -> 438 -0.15280
403 -> 440 0.15656
405 -> 438 0.13098
413 -> 437 -0.24774
414 -> 438 0.26835
415 -> 439 0.26027
416 -> 440 -0.23850
418 -> 440 -0.14293

Excited State 197: Singlet-A 4.2057 eV 294.80 nm f=0.0016 <S**2>=0.000

424 -> 441 0.13504

425 -> 441 0.47830

426 -> 443 0.48368

Excited State 198: Singlet-A 4.2136 eV 294.25 nm f=0.2458 <S**2>=0.000

428 -> 445 -0.10440

430 -> 448 0.20834

432 -> 452 0.28827

433 -> 451 0.36598

434 -> 451 0.15343

436 -> 462 -0.32765

Excited State 199: Singlet-A 4.2139 eV 294.23 nm f=0.0004 <S**2>=0.000

432 -> 450 0.27452

433 -> 449 0.41205

435 -> 464 -0.10898

436 -> 463 -0.34656

Excited State 200: Singlet-A 4.2242 eV 293.51 nm f=0.0031 <S**2>=0.000

417 -> 438 -0.11047

428 -> 446 0.10584

429 -> 445 -0.17658

430 -> 447 -0.19846

431 -> 446 -0.15806

432 -> 451 -0.18912

433 -> 452 -0.25668

434 -> 452 -0.11422

435 -> 458 -0.20036

435 -> 462 -0.22666

436 -> 457 0.10243

436 -> 465 0.31947

**Table S7.** Standard orientation of the optimized geometry for the closed-ring isomer of **[Ir(μ-Cl)(tBu-PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | 0.002235 | 2.10252 | 0.001335 |
| C | 0.068166 | 3.458041 | -1.500446 |
| C | 6.71318 | 2.338744 | 0.45859 |
| C | -6.707839 | 2.344271 | -0.460467 |
| N | -4.239989 | 2.745517 | -0.411599 |
| Cl | 0.00065 | -0.000013 | 1.68163 |
| C | -3.808985 | 1.411108 | 1.415913 |
| N | -2.056705 | 2.325491 | -0.351333 |
| N | 2.061597 | 2.323194 | 0.353796 |
| N | 4.24527 | 2.741599 | 0.413029 |
| O | 9.187823 | 4.781184 | -0.440068 |
| O | -9.181191 | 4.789727 | 0.434397 |
| C | -3.234452 | 2.049572 | 0.2368 |
| C | -5.167683 | 1.809333 | 1.489033 |
| C | -2.33145 | 3.227218 | -1.407577 |
| C | 1.188529 | 3.761046 | 2.113816 |
| C | 3.238842 | 2.04656 | -0.235019 |
| C | -5.524988 | 2.798581 | 0.349017 |
| C | 2.337512 | 3.224766 | 1.409842 |
| C | 1.211506 | 4.056147 | -2.061732 |
| C | -1.181721 | 3.763925 | -2.110068 |
| C | 5.170846 | 1.806231 | -1.489034 |
| C | 3.812032 | 1.40865 | -1.415062 |
| C | 5.529585 | 2.794813 | -0.348942 |
| C | 3.274533 | 0.574966 | -2.400251 |
| C | -1.204715 | 4.053642 | 2.06791 |
| C | 5.993208 | 1.385859 | -2.52526 |
| C | -3.272553 | 0.57684 | 2.401203 |
| C | -4.106098 | 0.153657 | 3.446047 |
| C | -5.692291 | 4.174775 | 0.947937 |
| C | -0.061904 | 3.456287 | 1.504728 |
| C | 5.696942 | 4.171519 | -0.946418 |
| C | 7.904434 | 2.976937 | 0.469232 |
| C | 1.132246 | 4.86665 | -3.201124 |
| C | -3.692214 | 3.501761 | -1.445479 |
| C | -5.990909 | 1.389169 | 2.524646 |
| C | 3.698549 | 3.49833 | 1.447121 |
| C | 9.115255 | 2.46938 | 1.282588 |
| C | -7.898259 | 2.983955 | -0.472869 |
| C | 4.107103 | 0.151792 | -3.445862 |
| C | -6.854389 | 4.857349 | 0.974293 |
| C | 6.859687 | 4.853046 | -0.973812 |
| C | 8.059962 | 4.238091 | -0.328309 |
| C | -4.478583 | 4.400378 | -2.31691 |
| C | 5.450308 | 0.5477 | -3.513536 |
| C | 4.48556 | 4.398668 | 2.315913 |
| C | -0.100846 | 5.108673 | -3.817165 |
| C | -1.124418 | 4.862126 | 3.208662 |
| C | 0.109187 | 5.102725 | 3.824272 |
| C | -5.449147 | 0.550245 | 3.51292 |
| C | -8.054061 | 4.244458 | 0.325748 |
| C | -1.259213 | 4.559541 | -3.266379 |
| C | 1.267023 | 4.554407 | 3.271606 |
| C | 8.753344 | 1.21242 | 2.106287 |
| C | 10.286185 | 2.098297 | 0.328288 |
| C | 4.349638 | 5.79554 | 2.19636 |
| C | 5.360843 | 3.881287 | 3.288719 |
| C | -6.986255 | 6.238726 | 1.650612 |
| C | -5.343952 | 3.880218 | -3.297101 |
| C | 9.584617 | 3.568476 | 2.278588 |
| C | -10.28048 | 2.104679 | -0.337679 |
| C | -7.502352 | 7.284991 | 0.62254 |
| C | 5.950797 | 6.128284 | 3.98738 |
| C | 5.077269 | 6.653158 | 3.026729 |
| C | -9.107997 | 2.478372 | -1.28902 |
| C | 6.992107 | 6.235228 | -1.648478 |
| C | 6.088569 | 4.741456 | 4.118136 |
| C | 5.628779 | 6.735043 | -2.183111 |
| C | -4.35111 | 5.797609 | -2.193482 |
| C | -7.97037 | 6.149135 | 2.851893 |
| C | -8.744257 | 1.223254 | -2.114686 |
| C | -9.575529 | 3.579971 | -2.283401 |
| C | -5.62325 | 6.735614 | 2.18832 |
| C | 7.974064 | 6.145905 | -2.8515 |
| C | 7.512048 | 7.279052 | -0.619569 |
| C | -5.077336 | 6.653045 | -3.027383 |
| C | -6.070216 | 4.738164 | -4.130118 |
| C | -5.940871 | 6.125477 | -3.995503 |
| Ir | -0.002447 | -2.101488 | 0.000216 |
| C | 0.061418 | -3.45588 | 1.503049 |
| C | 6.70686 | -2.34606 | -0.461239 |
| C | -6.713502 | -2.339591 | 0.458231 |
| N | -4.245568 | -2.740541 | 0.411569 |
| Cl | 0.000423 | 0.000928 | -1.680688 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.812875 | -1.407691 | -1.416578 | C | 1.259846 | -4.560214 | -3.2662 |
| N | -2.061974 | -2.321556 | 0.352482 | C | 8.741908 | -1.231542 | -2.123135 |
| N | 2.056535 | -2.325082 | -0.351861 | C | 10.280955 | -2.110455 | -0.347029 |
| N | 4.239448 | -2.746794 | -0.410117 | C | 4.352832 | -5.799361 | -2.188659 |
| O | 9.180833 | -4.788689 | 0.438725 | C | 5.342521 | -3.882926 | -3.296777 |
| O | -9.186277 | -4.784259 | -0.440274 | C | -6.989798 | -6.235635 | -1.649921 |
| C | -3.239269 | -2.045402 | -0.236562 | C | -5.352821 | -3.875533 | 3.295746 |
| C | -5.171592 | -1.805781 | -1.490461 | C | 9.5686 | -3.590228 | -2.286386 |
| C | -2.337904 | -3.223018 | 1.408705 | C | -10.28734 | -2.102453 | 0.334252 |
| C | 1.181901 | -3.763995 | -2.110334 | C | -7.507398 | -7.280168 | -0.620563 |
| C | 3.234015 | -2.049706 | 0.237029 | C | 5.941546 | -6.12879 | -3.991321 |
| C | -5.529922 | -2.794153 | -0.350217 | C | 5.079397 | -6.655543 | -3.021539 |
| C | 2.331447 | -3.227564 | -1.407367 | C | -9.114319 | -2.474444 | 1.285638 |
| C | 1.204018 | -4.054193 | 2.065627 | C | 6.9866 | -6.236179 | 1.657758 |
| C | -1.189051 | -3.760356 | 2.112094 | C | 6.069208 | -4.741576 | -4.128687 |
| C | 5.167466 | -1.806768 | 1.488252 | C | 5.624525 | -6.73167 | 2.199308 |
| C | 3.808565 | -1.409199 | 1.414976 | C | -4.358003 | -5.792475 | 2.19311 |
| C | 5.524587 | -2.798345 | 0.350317 | C | -7.972597 | -6.147753 | -2.852382 |
| C | 3.272182 | -0.573189 | 2.39879 | C | -8.752104 | -1.218753 | 2.111176 |
| C | -1.211551 | -4.054429 | -2.063889 | C | -9.580755 | -3.576184 | 2.280334 |
| C | 5.990955 | -1.384054 | 2.522608 | C | -5.626201 | -6.733484 | -2.185366 |
| C | -3.275633 | -0.574342 | -2.402201 | C | 7.973204 | -6.144262 | 2.856797 |
| C | -4.108337 | -0.151869 | -3.447993 | C | 7.500554 | -7.284835 | 0.630921 |
| C | -5.696397 | -4.170922 | -0.948003 | C | -5.085209 | -6.648253 | 3.025787 |
| C | -0.068261 | -3.456967 | -1.501768 | C | -6.079896 | -4.733826 | 4.127692 |
| C | 5.692023 | -4.173427 | 0.951853 | C | -5.950074 | -6.121081 | 3.992945 |
| C | 7.896877 | -2.986438 | -0.473947 | H | 6.837316 | 7.343219 | 0.242495 |
| C | 1.123457 | -4.863653 | 3.205665 | H | 8.511325 | 7.021098 | -0.265438 |
| C | -3.698864 | -3.496552 | 1.446078 | H | 7.554754 | 8.267352 | -1.092973 |
| C | -5.994042 | -1.386209 | -2.52695 | H | 8.970682 | 5.846546 | -2.523971 |
| C | 3.692131 | -3.502802 | -1.444298 | H | 7.61174 | 5.425018 | -3.594764 |
| C | 9.105384 | -2.484764 | -1.294383 | H | 8.044613 | 7.12599 | -3.338954 |
| C | -7.903954 | -2.979243 | 0.469719 | H | 5.763615 | 7.723875 | -2.634111 |
| C | 4.106026 | -0.147432 | 3.44235 | H | 5.222341 | 6.07321 | -2.957192 |
| C | -6.858577 | -4.853368 | -0.975345 | H | 4.886065 | 6.833507 | -1.382589 |
| C | 6.854032 | -4.856254 | 0.978575 | H | 7.945635 | 1.410758 | 2.820198 |
| C | 8.053269 | -4.244812 | 0.327865 | H | 8.44996 | 0.374951 | 1.467773 |
| C | -4.485999 | -4.395274 | 2.316623 | H | 9.633068 | 0.89379 | 2.675975 |
| C | 5.449265 | -0.543321 | 3.509411 | H | 10.406514 | 3.176625 | 2.889968 |
| C | 4.478555 | -4.402242 | -2.314895 | H | 9.938916 | 4.455075 | 1.750911 |
| C | -0.110218 | -5.104326 | 3.82108 | H | 8.768112 | 3.859593 | 2.949559 |
| C | -1.131891 | -4.865433 | -3.202896 | H | 11.127822 | 1.712991 | 0.91684 |
| C | 0.101553 | -5.108701 | -3.817748 | H | 9.982455 | 1.314749 | -0.376009 |
| C | -5.451435 | -0.548189 | -3.515497 | H | 10.623685 | 2.968991 | -0.235125 |
| C | -8.059187 | -4.239356 | -0.329716 | H | 9.982426 | -1.320644 | 0.352421 |
| C | -1.267839 | -4.554893 | 3.269053 | H | 10.617569 | -2.978154 | 0.221483 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 11.121862 | -1.732508 | -0.9414 | H | -2.227557 | -4.742962 | 3.736715 |
| H | 8.439616 | -0.391197 | -1.487874 | H | 5.221486 | -6.06534 | 2.9713 |
| H | 9.620606 | -0.915361 | -2.69573 | H | 4.879032 | -6.833484 | 1.401789 |
| H | 7.932893 | -1.433231 | -2.834618 | H | 5.759844 | -7.718324 | 2.654959 |
| H | 9.926081 | -4.473372 | -1.755039 | H | 7.613798 | -5.421618 | 3.599771 |
| H | 8.748025 | -3.886193 | -2.95027 | H | 8.045384 | -7.123273 | 3.346125 |
| H | 10.38638 | -3.202247 | -2.905687 | H | 8.968682 | -5.845963 | 2.524839 |
| H | -10.40128 | -3.186339 | 2.894848 | H | 7.543233 | -8.271439 | 1.107906 |
| H | -9.935596 | -4.461709 | 1.751235 | H | 6.822433 | -7.350867 | -0.228334 |
| H | -8.762583 | -3.86874 | 2.948652 | H | 8.49907 | -7.03031 | 0.272183 |
| H | -9.986808 | -1.314655 | -0.366654 | H | -6.551898 | -1.425655 | 1.017411 |
| H | -10.6225 | -2.971491 | -0.233039 | H | -4.797946 | -4.562047 | -1.410142 |
| H | -11.12956 | -1.722498 | 0.925429 | H | -4.794508 | 4.565304 | 1.411929 |
| H | -7.942384 | -1.417577 | 2.822666 | H | -6.545891 | 1.430312 | -1.019526 |
| H | -8.451261 | -0.379566 | 1.473659 | H | 6.550869 | 1.424798 | 1.017541 |
| H | -9.6308 | -0.902392 | 2.683629 | H | 4.798817 | 4.56338 | -1.408526 |
| H | -8.439373 | 0.385334 | -1.477452 | H | 5.451976 | 2.806023 | 3.401151 |
| H | -9.623618 | 0.904039 | -2.684583 | H | 6.753591 | 4.329918 | 4.87081 |
| H | -7.936959 | 1.424015 | -2.828407 | H | 6.514276 | 6.794514 | 4.632615 |
| H | -10.61658 | 2.973073 | 0.230053 | H | 4.960307 | 7.727403 | 2.926493 |
| H | -11.12248 | 1.724466 | -0.929028 | H | 3.663381 | 6.199812 | 1.459655 |
| H | -9.97901 | 1.316596 | 0.36251 | H | 2.226702 | 4.742412 | 3.73939 |
| H | -9.932921 | 4.464326 | -1.754047 | H | 0.169151 | 5.712911 | 4.719976 |
| H | -8.757145 | 3.874948 | -2.950401 | H | -2.03044 | 5.298063 | 3.621794 |
| H | -10.39439 | 3.188866 | -2.899308 | H | -2.177698 | 3.882543 | 1.626555 |
| H | -8.040337 | 7.128598 | 3.340719 | H | 2.235111 | -0.267662 | 2.355356 |
| H | -8.966853 | 5.851756 | 2.522172 | H | 3.693159 | 0.492507 | 4.215112 |
| H | -7.610337 | 5.426583 | 3.59465 | H | 6.072462 | -0.214661 | 4.334903 |
| H | -7.544789 | 8.272444 | 1.09775 | H | 7.024366 | -1.710014 | 2.578614 |
| H | -6.825421 | 7.349686 | -0.237773 | H | 2.237557 | 0.269269 | -2.356338 |
| H | -8.501142 | 7.028986 | 0.265742 | H | 3.693209 | -0.486065 | -4.21981 |
| H | -5.75756 | 7.723798 | 2.640962 | H | 6.072533 | 0.220975 | -4.340517 |
| H | -5.218571 | 6.071954 | 2.961675 | H | 7.026647 | 1.711699 | -2.5815 |
| H | -4.879334 | 6.834423 | 1.388907 | H | -2.184447 | -3.881601 | -1.623024 |
| H | -8.50693 | -7.023783 | -0.265968 | H | -2.038291 | -5.301392 | -3.61518 |
| H | -7.548822 | -8.268653 | -1.093725 | H | 0.161059 | -5.721139 | -4.711945 |
| H | -6.83218 | -7.343074 | 0.241215 | H | 2.219408 | -4.750387 | -3.733336 |
| H | -4.883717 | -6.833884 | -1.384863 | H | 3.675062 | -6.205219 | -1.445002 |
| H | -5.760654 | -7.721125 | -2.639132 | H | 4.970288 | -7.730123 | -2.916197 |
| H | -5.219822 | -6.06936 | -2.957511 | H | 6.504111 | -6.793896 | -4.638514 |
| H | -7.611086 | -5.427359 | -3.596506 | H | 6.725443 | -4.328727 | -4.888322 |
| H | -8.042973 | -7.128345 | -3.338835 | H | 5.425782 | -2.807497 | -3.413832 |
| H | -8.969271 | -5.848932 | -2.524517 | H | -5.428421 | 2.804678 | -3.412202 |
| H | 2.177053 | -3.883157 | 1.624336 | H | -3.67219 | 6.204078 | -1.451215 |
| H | 2.029314 | -5.300372 | 3.618334 | H | -4.96689 | 7.727696 | -2.924165 |
| H | -0.170414 | -5.71543 | 4.716144 | H | -6.503157 | 6.79001 | -4.64353 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -6.727464 | 4.324645 | -4.888509 | H | -2.235705 | 0.270599 | 2.357832 |
| H | -2.218499 | 4.74873 | -3.734462 | H | -3.693149 | -0.484779 | 4.220015 |
| H | -0.160026 | 5.720629 | -4.711714 | H | -6.072147 | 0.223412 | 4.339288 |
| H | 2.038677 | 5.303124 | -3.612793 | H | -7.024192 | 1.715589 | 2.580329 |
| H | 2.184147 | 3.884129 | -1.619937 | H | -7.027321 | -1.712547 | -2.583178 |
| H | -3.678149 | -6.19862 | 1.451516 | H | -2.238742 | -0.268354 | -2.358434 |
| H | -4.974471 | -7.722856 | 2.922389 | H | -3.694656 | 0.485774 | -4.222228 |
| H | -6.513015 | -6.785874 | 4.640136 | H | -6.073745 | -0.222018 | -4.342645 |
| H | -6.738206 | -4.320604 | 4.885323 | H | 4.794514 | -4.562725 | 1.417341 |
| H | -5.437715 | -2.800049 | 3.411002 | H | 6.544485 | -1.433506 | -1.02244 |

The Result for the TDDFT calculation

Excited State 1: Singlet-A 2.0448 eV 606.35 nm f=0.0000 <S**2>=0.000

563 -> 565 -0.20285

563 -> 567 -0.11191

564 -> 565 0.66142

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -7281.48422413

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.0912 eV 592.90 nm f=0.0000 <S**2>=0.000

563 -> 565 -0.14423

563 -> 566 0.20914

563 -> 568 -0.10496

564 -> 566 0.63132

564 -> 567 0.13299

Excited State 3: Singlet-A 2.1032 eV 589.50 nm f=0.0000 <S**2>=0.000

563 -> 565 -0.24107

563 -> 567 0.19379

564 -> 566 -0.16953

564 -> 567 0.59633

Excited State 4: Singlet-A 2.1368 eV 580.23 nm f=0.0001 <S**2>=0.000

563 -> 566 -0.23547

563 -> 568 -0.19623

564 -> 568 0.62616

Excited State 5: Singlet-A 2.1950 eV 564.86 nm f=0.0003 <S**2>=0.000
563 -> 565 0.61290
564 -> 565 0.18461
564 -> 567 0.27380

Excited State 6: Singlet-A 2.2391 eV 553.72 nm f=0.0002 <S**2>=0.000
563 -> 566 0.60760
563 -> 567 0.17271
564 -> 566 -0.20483
564 -> 568 0.20974

Excited State 7: Singlet-A 2.2490 eV 551.28 nm f=0.0002 <S**2>=0.000
563 -> 566 -0.14715
563 -> 567 0.63563
564 -> 565 0.10401
564 -> 567 -0.20618
564 -> 568 -0.11740

Excited State 8: Singlet-A 2.2885 eV 541.77 nm f=0.0003 <S**2>=0.000
563 -> 568 0.65987
564 -> 566 0.11453
564 -> 568 0.21424

Excited State 9: Singlet-A 2.5766 eV 481.18 nm f=0.0012 <S**2>=0.000
562 -> 565 0.69974

Excited State 10: Singlet-A 2.6156 eV 474.01 nm f=0.0111 <S**2>=0.000
562 -> 566 -0.10224
563 -> 571 0.16194
564 -> 569 0.67169

Excited State 11: Singlet-A 2.6251 eV 472.31 nm f=0.0003 <S**2>=0.000
562 -> 566 0.69005

Excited State 12: Singlet-A 2.6427 eV 469.16 nm f=0.0002 <S**2>=0.000

562 -> 567 0.69734

Excited State 13: Singlet-A 2.6747 eV 463.55 nm f=0.0017 <S**2>=0.000
558 -> 565 -0.16041
559 -> 565 0.25025
559 -> 567 0.10331
560 -> 565 0.16913
561 -> 565 0.50383
562 -> 568 -0.18204
563 -> 569 -0.18517
564 -> 571 -0.11986

Excited State 14: Singlet-A 2.6777 eV 463.02 nm f=0.0003 <S**2>=0.000
561 -> 565 0.18806
562 -> 568 0.64728

Excited State 15: Singlet-A 2.6835 eV 462.02 nm f=0.0108 <S**2>=0.000
561 -> 565 0.16532
562 -> 568 -0.14905
563 -> 569 0.54223
564 -> 571 0.35952

Excited State 16: Singlet-A 2.6877 eV 461.30 nm f=0.0206 <S**2>=0.000
562 -> 568 -0.11730
563 -> 572 -0.17249
564 -> 570 0.66454

Excited State 17: Singlet-A 2.7229 eV 455.33 nm f=0.0001 <S**2>=0.000
558 -> 567 -0.15167
559 -> 565 0.20005
559 -> 567 -0.22632
560 -> 565 0.33905
560 -> 567 -0.12757
561 -> 565 -0.19980
561 -> 566 0.17061
561 -> 567 0.39043

Excited State 18: Singlet-A 2.7364 eV 453.10 nm f=0.0007 <S**2>=0.000

| | |
|---|---|
| 558 -> 566 | 0.16504 |
| 559 -> 566 | -0.25311 |
| 559 -> 568 | 0.11071 |
| 560 -> 565 | -0.14111 |
| 560 -> 566 | 0.18674 |
| 561 -> 566 | 0.50946 |
| 561 -> 567 | -0.10698 |
| 563 -> 570 | -0.14065 |
| 564 -> 572 | 0.10490 |

Excited State 19: Singlet-A 2.7493 eV 450.97 nm f=0.0078 <S**2>=0.000

| | |
|---|---|
| 560 -> 565 | 0.25424 |
| 561 -> 566 | 0.15351 |
| 561 -> 567 | -0.22733 |
| 563 -> 570 | 0.43765 |
| 564 -> 572 | -0.32469 |

Excited State 20: Singlet-A 2.7508 eV 450.71 nm f=0.0026 <S**2>=0.000

| | |
|---|---|
| 559 -> 565 | -0.13398 |
| 560 -> 565 | 0.50482 |
| 561 -> 567 | -0.23745 |
| 563 -> 570 | -0.29213 |
| 564 -> 572 | 0.21985 |

Excited State 21: Singlet-A 2.7742 eV 446.92 nm f=0.0007 <S**2>=0.000

| | |
|---|---|
| 558 -> 568 | 0.15751 |
| 559 -> 566 | 0.16994 |
| 559 -> 568 | 0.21692 |
| 560 -> 566 | -0.30782 |
| 560 -> 568 | -0.14336 |
| 561 -> 566 | 0.15788 |
| 561 -> 568 | 0.45985 |
| 563 -> 570 | -0.10004 |

Excited State 22: Singlet-A 2.7978 eV 443.14 nm f=0.0002 <S**2>=0.000
559 -> 566 0.12816
560 -> 566 0.58485
560 -> 567 0.14875
561 -> 568 0.27199

Excited State 23: Singlet-A 2.8081 eV 441.52 nm f=0.0001 <S**2>=0.000
560 -> 566 -0.11939
560 -> 567 0.65634
561 -> 565 -0.10235
561 -> 567 0.12949
561 -> 568 -0.10451

Excited State 24: Singlet-A 2.8260 eV 438.73 nm f=0.0025 <S**2>=0.000
563 -> 569 -0.38186
564 -> 571 0.58602

Excited State 25: Singlet-A 2.8452 eV 435.77 nm f=0.0003 <S**2>=0.000
560 -> 568 0.67205
561 -> 566 0.10131
561 -> 568 0.15885

Excited State 26: Singlet-A 2.8688 eV 432.18 nm f=0.0005 <S**2>=0.000
559 -> 565 0.56929
559 -> 567 0.11632
561 -> 565 -0.24482
561 -> 567 -0.27198

Excited State 27: Singlet-A 2.8867 eV 429.50 nm f=0.0015 <S**2>=0.000
563 -> 570 0.41807
564 -> 572 0.56025

Excited State 28: Singlet-A 2.8927 eV 428.61 nm f=0.0005 <S**2>=0.000
563 -> 571 0.67365
564 -> 569 -0.16544

Excited State 29: Singlet-A 2.9143 eV 425.44 nm f=0.0006 <S**2>=0.000

556 -> 567 0.10065

559 -> 566 0.33723

559 -> 567 0.49927

561 -> 565 -0.15843

561 -> 566 0.14706

561 -> 567 0.23667

Excited State 30: Singlet-A 2.9243 eV 423.98 nm f=0.0003 <S**2>=0.000

559 -> 566 0.47937

559 -> 567 -0.33759

559 -> 568 -0.10345

561 -> 566 0.21887

561 -> 567 -0.16045

561 -> 568 -0.22452

Excited State 31: Singlet-A 2.9495 eV 420.36 nm f=0.0003 <S**2>=0.000

563 -> 572 0.67212

564 -> 570 0.17804

Excited State 32: Singlet-A 2.9685 eV 417.67 nm f=0.0006 <S**2>=0.000

556 -> 568 -0.10721

559 -> 568 0.62017

561 -> 566 -0.13861

561 -> 568 -0.25831

Excited State 33: Singlet-A 3.0123 eV 411.59 nm f=0.0000 <S**2>=0.000

556 -> 565 -0.14764

557 -> 565 0.17304

558 -> 565 0.62116

561 -> 565 0.16795

Excited State 34: Singlet-A 3.0499 eV 406.52 nm f=0.0001 <S**2>=0.000

557 -> 565 0.59054

558 -> 565 -0.19118

558 -> 566 0.16406

558 -> 567 0.19919

Excited State 35: Singlet-A 3.0579 eV 405.46 nm f=0.0002 <S**2>=0.000
556 -> 566 0.19211
557 -> 565 -0.15467
558 -> 566 0.60129
561 -> 566 -0.16779

Excited State 36: Singlet-A 3.0761 eV 403.05 nm f=0.0154 <S**2>=0.000
556 -> 565 -0.15728
557 -> 565 -0.22910
557 -> 567 -0.13180
558 -> 567 0.46850
561 -> 567 0.11665
562 -> 569 0.37187

Excited State 37: Singlet-A 3.0797 eV 402.58 nm f=0.0398 <S**2>=0.000
557 -> 565 0.15791
558 -> 567 -0.30972
562 -> 569 0.57230

Excited State 38: Singlet-A 3.0991 eV 400.06 nm f=0.0001 <S**2>=0.000
556 -> 566 -0.22861
556 -> 568 -0.15843
557 -> 566 -0.31875
558 -> 566 0.10972
558 -> 568 0.50395
561 -> 568 -0.16796

Excited State 39: Singlet-A 3.1123 eV 398.37 nm f=0.0004 <S**2>=0.000
557 -> 566 0.56442
557 -> 567 0.21915
558 -> 568 0.30902

Excited State 40: Singlet-A 3.1213 eV 397.22 nm f=0.0002 <S**2>=0.000
557 -> 566 -0.20187

557 -> 567 0.63597
558 -> 567 0.13012
558 -> 568 -0.11912

Excited State 41: Singlet-A 3.1434 eV 394.43 nm f=0.0010 <S**2>=0.000
555 -> 565 0.45136
556 -> 565 0.45166
556 -> 567 0.11811
558 -> 567 0.15610

Excited State 42: Singlet-A 3.1626 eV 392.04 nm f=0.0004 <S**2>=0.000
556 -> 568 0.11844
557 -> 568 0.64220
562 -> 570 -0.22249

Excited State 43: Singlet-A 3.1718 eV 390.90 nm f=0.0077 <S**2>=0.000
555 -> 565 -0.10907
555 -> 566 0.17659
556 -> 565 0.14544
556 -> 566 -0.15295
557 -> 568 0.18346
562 -> 570 0.56161

Excited State 44: Singlet-A 3.1782 eV 390.10 nm f=0.0019 <S**2>=0.000
555 -> 565 0.32323
555 -> 566 -0.21615
555 -> 567 -0.16573
556 -> 565 -0.26878
556 -> 566 0.24171
556 -> 567 0.16134
558 -> 566 -0.10087
558 -> 567 -0.10804
562 -> 570 0.29913

Excited State 45: Singlet-A 3.1869 eV 389.04 nm f=0.0012 <S**2>=0.000
555 -> 565 -0.22155

555 -> 566 -0.29386
555 -> 567 0.21177
556 -> 565 0.19557
556 -> 566 0.35669
556 -> 567 -0.22295
558 -> 566 -0.10772
558 -> 567 0.12354
558 -> 568 0.14221

Excited State 46: Singlet-A 3.2024 eV 387.16 nm f=0.0006 <S**2>=0.000
557 -> 569 -0.10967
560 -> 569 -0.37344
562 -> 571 0.56360

Excited State 47: Singlet-A 3.2071 eV 386.60 nm f=0.0001 <S**2>=0.000
545 -> 565 0.39845
545 -> 567 0.16787
547 -> 565 -0.39104
547 -> 567 -0.13142
548 -> 565 -0.25272

Excited State 48: Singlet-A 3.2181 eV 385.27 nm f=0.0010 <S**2>=0.000
555 -> 566 0.35037
555 -> 568 0.28236
556 -> 566 0.27743
556 -> 568 0.36231
558 -> 568 0.20513

Excited State 49: Singlet-A 3.2254 eV 384.40 nm f=0.0001 <S**2>=0.000
555 -> 565 -0.33097
555 -> 567 -0.31912
556 -> 565 0.22950
556 -> 567 0.40720
558 -> 565 0.11385

Excited State 50: Singlet-A 3.2454 eV 382.02 nm f=0.0002 <S**2>=0.000

544 -> 566 -0.16537
546 -> 566 0.27896
546 -> 568 -0.10774
547 -> 566 -0.34410
547 -> 568 0.12760
548 -> 566 0.38253
548 -> 568 -0.13644
556 -> 566 0.10267

Excited State 51: Singlet-A 3.2477 eV 381.76 nm f=0.0003 <S**2>=0.000
544 -> 567 0.12723
545 -> 565 -0.17712
545 -> 567 0.37439
546 -> 567 0.22782
547 -> 565 -0.10040
547 -> 567 0.23905
548 -> 567 0.18966
556 -> 567 0.22931
560 -> 569 0.12110

Excited State 52: Singlet-A 3.2509 eV 381.38 nm f=0.0039 <S**2>=0.000
545 -> 567 -0.12062
560 -> 569 0.46825
562 -> 571 0.25072
562 -> 572 0.36194

Excited State 53: Singlet-A 3.2556 eV 380.83 nm f=0.0002 <S**2>=0.000
555 -> 566 0.39822
555 -> 567 0.22863
555 -> 568 -0.20087
556 -> 566 0.23136
556 -> 567 0.14944
556 -> 568 -0.29470
558 -> 566 -0.11152

Excited State 54: Singlet-A 3.2640 eV 379.85 nm f=0.0002 <S**2>=0.000

555 -> 566 -0.16633
555 -> 567 0.47822
555 -> 568 0.14032
556 -> 567 0.31979
556 -> 568 0.22325
558 -> 567 -0.10999

Excited State 55: Singlet-A 3.2911 eV 376.73 nm f=0.0036 <S**2>=0.000
555 -> 568 0.14885
556 -> 568 -0.12082
560 -> 569 0.24601
560 -> 570 0.40851
562 -> 571 0.22638
562 -> 572 -0.37202

Excited State 56: Singlet-A 3.2930 eV 376.51 nm f=0.0001 <S**2>=0.000
543 -> 568 0.20756
544 -> 566 0.16923
544 -> 568 0.44033
546 -> 568 -0.14093
547 -> 568 -0.12743
548 -> 568 0.17796
555 -> 568 -0.16137
556 -> 568 0.18917
560 -> 570 0.10192
562 -> 572 -0.10870

Excited State 57: Singlet-A 3.2982 eV 375.91 nm f=0.0002 <S**2>=0.000
543 -> 568 0.10297
544 -> 568 0.21090
555 -> 568 0.53741
556 -> 568 -0.26857

Excited State 58: Singlet-A 3.3355 eV 371.71 nm f=0.0086 <S**2>=0.000
560 -> 569 -0.15662
560 -> 570 0.51615

562 -> 572 0.37217
564 -> 573 0.13502

Excited State 59: Singlet-A 3.3544 eV 369.62 nm f=0.0001 <S**2>=0.000
559 -> 569 -0.10621
560 -> 570 -0.12908
563 -> 574 0.13636
563 -> 575 -0.16900
563 -> 578 0.10496
564 -> 573 0.58904

Excited State 60: Singlet-A 3.3629 eV 368.69 nm f=0.0006 <S**2>=0.000
553 -> 565 0.17638
553 -> 567 0.10535
554 -> 565 0.66221

Excited State 61: Singlet-A 3.3691 eV 368.00 nm f=0.0111 <S**2>=0.000
560 -> 571 0.40849
560 -> 572 -0.13885
561 -> 569 0.43327
563 -> 573 0.19182
564 -> 574 0.10805
564 -> 575 -0.15153

Excited State 62: Singlet-A 3.3980 eV 364.88 nm f=0.0015 <S**2>=0.000
560 -> 571 -0.19523
560 -> 572 0.13378
561 -> 569 0.50780
563 -> 573 -0.24008
564 -> 574 -0.18653
564 -> 575 0.21056

Excited State 63: Singlet-A 3.4094 eV 363.66 nm f=0.0010 <S**2>=0.000
553 -> 566 -0.19101
553 -> 568 0.10795
554 -> 566 0.64880

Excited State 64: Singlet-A 3.4160 eV 362.96 nm f=0.1337 <S**2>=0.000

560 -> 571 0.45082
560 -> 572 0.18492
561 -> 569 -0.14183
561 -> 570 0.11243
563 -> 573 -0.27002
564 -> 574 -0.26009
564 -> 578 -0.13465

Excited State 65: Singlet-A 3.4226 eV 362.25 nm f=0.0001 <S**2>=0.000

553 -> 565 0.21836
553 -> 567 -0.17839
554 -> 567 0.63162

Excited State 66: Singlet-A 3.4499 eV 359.39 nm f=0.1131 <S**2>=0.000

555 -> 570 -0.10254
560 -> 572 0.49900
561 -> 570 0.33239
563 -> 573 0.15364
564 -> 574 0.13911
564 -> 575 -0.19251

Excited State 67: Singlet-A 3.4549 eV 358.86 nm f=0.0081 <S**2>=0.000

553 -> 566 0.20245
553 -> 568 0.17611
554 -> 568 0.62422

Excited State 68: Singlet-A 3.4603 eV 358.31 nm f=0.0625 <S**2>=0.000

558 -> 570 0.11654
559 -> 569 0.10891
560 -> 572 -0.21815
561 -> 570 0.52416
563 -> 576 0.13669
564 -> 574 0.16393
564 -> 575 0.24443

Excited State 69: Singlet-A 3.4653 eV 357.78 nm f=0.0489 <S**2>=0.000

554 -> 568 -0.10569

559 -> 569 0.61026

561 -> 570 -0.11975

564 -> 573 0.12480

564 -> 576 0.16326

Excited State 70: Singlet-A 3.4780 eV 356.48 nm f=0.0115 <S**2>=0.000

559 -> 569 -0.24390

563 -> 575 0.21480

563 -> 579 -0.11262

564 -> 574 0.12303

564 -> 575 0.17678

564 -> 576 0.49682

564 -> 577 0.17009

Excited State 71: Singlet-A 3.4974 eV 354.51 nm f=0.0037 <S**2>=0.000

560 -> 571 0.14282

560 -> 572 0.22415

561 -> 570 -0.22734

563 -> 576 0.19636

564 -> 574 0.40867

564 -> 575 0.27727

564 -> 576 -0.22824

Excited State 72: Singlet-A 3.5340 eV 350.83 nm f=0.0002 <S**2>=0.000

553 -> 565 0.63490

554 -> 565 -0.16403

554 -> 567 -0.23234

Excited State 73: Singlet-A 3.5380 eV 350.43 nm f=0.0494 <S**2>=0.000

557 -> 570 0.11151

559 -> 570 0.62222

561 -> 572 0.13638

563 -> 574 -0.10359

564 -> 577 0.12464

Excited State 74: Singlet-A 3.5403 eV 350.21 nm f=0.0296 <S**2>=0.000
560 -> 572 0.12920
563 -> 573 0.32905
563 -> 576 0.10992
563 -> 577 0.23682
564 -> 574 -0.32722
564 -> 575 0.23023
564 -> 577 -0.10369
564 -> 578 0.25129
564 -> 579 -0.15156

Excited State 75: Singlet-A 3.5451 eV 349.73 nm f=0.0211 <S**2>=0.000
557 -> 569 -0.23354
558 -> 571 -0.12008
561 -> 571 0.62698

Excited State 76: Singlet-A 3.5746 eV 346.84 nm f=0.0140 <S**2>=0.000
557 -> 569 0.18847
559 -> 570 -0.20726
563 -> 574 -0.36516
563 -> 578 0.16494
563 -> 579 -0.12772
564 -> 576 -0.12043
564 -> 577 0.40334
564 -> 578 0.15457

Excited State 77: Singlet-A 3.5785 eV 346.47 nm f=0.0002 <S**2>=0.000
553 -> 566 0.62756
553 -> 567 0.11366
554 -> 566 0.18621
554 -> 568 -0.18772

Excited State 78: Singlet-A 3.5860 eV 345.75 nm f=0.0045 <S**2>=0.000
553 -> 567 -0.11236

559 -> 571 -0.10219
563 -> 573 0.31403
563 -> 577 -0.19868
564 -> 575 0.28432
564 -> 578 -0.13063
564 -> 579 0.40568

Excited State 79: Singlet-A 3.5896 eV 345.40 nm f=0.0015 <S**2>=0.000
553 -> 566 -0.10363
553 -> 567 0.63667
554 -> 565 -0.10001
554 -> 567 0.17706
557 -> 569 -0.11383

Excited State 80: Singlet-A 3.5912 eV 345.24 nm f=0.0290 <S**2>=0.000
553 -> 567 0.12429
557 -> 569 0.57225
561 -> 571 0.22210
562 -> 571 0.10045
563 -> 574 0.16407
564 -> 577 -0.10025

Excited State 81: Singlet-A 3.5981 eV 344.58 nm f=0.0003 <S**2>=0.000
555 -> 569 -0.10847
558 -> 569 -0.34681
559 -> 571 0.54213
564 -> 578 -0.10996

Excited State 82: Singlet-A 3.6008 eV 344.32 nm f=0.0012 <S**2>=0.000
558 -> 569 0.10823
559 -> 571 -0.10817
563 -> 574 0.41282
563 -> 575 -0.22060
563 -> 578 0.18453
563 -> 579 -0.11690
564 -> 573 -0.23575

564 -> 577 0.18716
564 -> 580 -0.12500
564 -> 581 -0.18284

Excited State 83: Singlet-A 3.6078 eV 343.65 nm f=0.0195 <S**2>=0.000
556 -> 570 0.11843
557 -> 570 0.12416
558 -> 572 0.14061
559 -> 570 -0.10881
561 -> 572 0.63492

Excited State 84: Singlet-A 3.6173 eV 342.75 nm f=0.0196 <S**2>=0.000
555 -> 569 -0.11622
558 -> 569 -0.29443
563 -> 573 -0.20547
563 -> 575 -0.15898
563 -> 576 -0.17297
563 -> 580 -0.13220
564 -> 577 -0.10520
564 -> 578 0.40383
564 -> 579 0.20884

Excited State 85: Singlet-A 3.6286 eV 341.68 nm f=0.0001 <S**2>=0.000
553 -> 568 0.66687
554 -> 566 -0.10928
554 -> 568 -0.19250

Excited State 86: Singlet-A 3.6314 eV 341.42 nm f=0.0021 <S**2>=0.000
555 -> 569 0.17713
557 -> 571 0.11896
558 -> 569 0.30187
559 -> 571 0.28099
563 -> 574 -0.12472
563 -> 575 -0.30088
564 -> 575 0.12527
564 -> 576 0.14828

564 -> 578 0.12093
564 -> 580 -0.24964

Excited State 87: Singlet-A 3.6358 eV 341.01 nm f=0.0043 <S**2>=0.000
555 -> 569 0.14152
558 -> 569 0.21178
559 -> 571 0.22603
563 -> 574 0.14943
563 -> 575 0.23099
563 -> 576 -0.19456
563 -> 579 -0.12311
564 -> 576 -0.20276
564 -> 578 0.22150
564 -> 579 0.11688
564 -> 580 0.30071
564 -> 581 -0.11012

Excited State 88: Singlet-A 3.6621 eV 338.56 nm f=0.0016 <S**2>=0.000
563 -> 575 0.32544
563 -> 576 0.28311
563 -> 578 0.15298
563 -> 579 0.19694
563 -> 580 -0.15200
564 -> 575 -0.13440
564 -> 579 0.24519
564 -> 580 -0.31535

Excited State 89: Singlet-A 3.6649 eV 338.30 nm f=0.0012 <S**2>=0.000
557 -> 570 -0.11923
563 -> 575 -0.17417
563 -> 576 0.42809
563 -> 578 -0.17748
563 -> 579 -0.14252
563 -> 580 -0.15238
564 -> 576 0.12683
564 -> 579 0.21663

564 -> 580 0.28589

Excited State 90: Singlet-A 3.6702 eV 337.82 nm f=0.0059 <S**2>=0.000
555 -> 570 -0.10525
558 -> 570 -0.37310
559 -> 572 0.56223

Excited State 91: Singlet-A 3.6807 eV 336.85 nm f=0.0162 <S**2>=0.000
557 -> 570 0.59940
558 -> 571 0.11661
561 -> 572 -0.18699
563 -> 575 -0.11218

Excited State 92: Singlet-A 3.6952 eV 335.53 nm f=0.0001 <S**2>=0.000
555 -> 570 0.24653
557 -> 571 0.14586
557 -> 572 0.22188
558 -> 570 0.44455
559 -> 572 0.33216
560 -> 572 0.13835
561 -> 570 -0.11461

Excited State 93: Singlet-A 3.7232 eV 333.01 nm f=0.0040 <S**2>=0.000
563 -> 574 0.17722
563 -> 582 0.19480
563 -> 583 -0.11054
564 -> 577 0.20758
564 -> 581 0.56526

Excited State 94: Singlet-A 3.7297 eV 332.42 nm f=0.0162 <S**2>=0.000
555 -> 569 0.52572
556 -> 571 -0.13527
557 -> 571 0.24382
558 -> 569 -0.32203

Excited State 95: Singlet-A 3.7499 eV 330.63 nm f=0.0573 <S**2>=0.000

555 -> 569 0.10647
557 -> 571 -0.27197
563 -> 577 0.22625
563 -> 578 0.12477
563 -> 581 0.26315
564 -> 582 0.42737
564 -> 583 -0.21044

Excited State 96: Singlet-A 3.7601 eV 329.74 nm f=0.0034 <S**2>=0.000
556 -> 569 -0.10711
563 -> 575 -0.10990
563 -> 577 -0.10175
563 -> 578 0.33322
563 -> 579 0.23022
563 -> 584 0.11832
564 -> 576 0.12006
564 -> 580 0.26614
564 -> 582 0.15810
564 -> 583 0.36406

Excited State 97: Singlet-A 3.7622 eV 329.55 nm f=0.1143 <S**2>=0.000
555 -> 569 -0.25936
555 -> 570 -0.10067
556 -> 569 -0.11312
557 -> 571 0.47990
558 -> 570 -0.11945
559 -> 572 -0.10637
563 -> 577 0.13643
563 -> 581 0.11132
564 -> 582 0.17347
564 -> 583 -0.15252

Excited State 98: Singlet-A 3.7646 eV 329.35 nm f=0.0769 <S**2>=0.000
556 -> 569 0.59015
557 -> 571 0.10653
558 -> 571 0.28924

Excited State 99: Singlet-A 3.7860 eV 327.48 nm f=0.0077 <S**2>=0.000

555 -> 571 0.33359
556 -> 569 -0.23971
558 -> 571 0.40291
558 -> 572 -0.12872
563 -> 578 -0.20761
564 -> 577 0.12523
564 -> 581 -0.13806

Excited State 100: Singlet-A 3.7956 eV 326.66 nm f=0.0052 <S**2>=0.000

555 -> 570 0.20299
558 -> 571 0.13768
563 -> 577 0.15067
563 -> 578 0.29050
563 -> 579 -0.11378
563 -> 580 -0.29016
563 -> 581 -0.13040
563 -> 583 -0.12162
563 -> 584 -0.10905
564 -> 578 -0.22075
564 -> 582 -0.18813
564 -> 583 -0.14207

Excited State 101: Singlet-A 3.7985 eV 326.40 nm f=0.0048 <S**2>=0.000

555 -> 570 0.22924
558 -> 570 -0.10347
558 -> 571 -0.13479
558 -> 572 0.10070
563 -> 577 0.29940
563 -> 578 -0.21822
563 -> 579 0.17053
563 -> 580 -0.23323
563 -> 584 0.11292
564 -> 577 0.23977
564 -> 581 -0.13594

564 -> 583 0.18120

Excited State 102: Singlet-A 3.8006 eV 326.22 nm f=0.0040 <S**2>=0.000
555 -> 570 0.41355
556 -> 572 0.14286
557 -> 572 0.18216
558 -> 570 -0.26314
563 -> 580 0.20250
563 -> 583 0.16990
564 -> 584 0.24127

Excited State 103: Singlet-A 3.8068 eV 325.69 nm f=0.0017 <S**2>=0.000
555 -> 570 -0.15916
557 -> 572 -0.11365
558 -> 570 0.11368
563 -> 577 0.25296
563 -> 579 -0.10767
563 -> 581 -0.15324
563 -> 582 0.15202
563 -> 583 0.21994
564 -> 578 -0.12005
564 -> 579 0.12406
564 -> 583 0.12220
564 -> 584 0.42357

Excited State 104: Singlet-A 3.8107 eV 325.36 nm f=0.0084 <S**2>=0.000
557 -> 572 -0.10515
563 -> 577 0.22585
563 -> 579 -0.14265
563 -> 580 0.42142
563 -> 583 -0.10309
564 -> 579 0.25753
564 -> 583 0.13290
564 -> 584 -0.30489

Excited State 105: Singlet-A 3.8145 eV 325.04 nm f=0.0031 <S**2>=0.000

558 -> 572 0.11147
563 -> 579 0.41062
563 -> 580 0.21378
563 -> 584 -0.21908
564 -> 577 0.11110
564 -> 580 0.20687
564 -> 582 -0.18914
564 -> 583 -0.26532

Excited State 106: Singlet-A 3.8296 eV 323.75 nm f=0.0781 <S**2>=0.000
556 -> 570 0.60514
558 -> 572 -0.22572
563 -> 579 0.12244
564 -> 581 -0.11533

Excited State 107: Singlet-A 3.8329 eV 323.48 nm f=0.0396 <S**2>=0.000
555 -> 569 0.10811
555 -> 570 -0.27378
557 -> 572 0.55243
563 -> 577 0.15648

Excited State 108: Singlet-A 3.8437 eV 322.56 nm f=0.0082 <S**2>=0.000
555 -> 572 0.34824
556 -> 570 0.19859
557 -> 570 -0.16605
558 -> 571 0.14059
558 -> 572 0.43739
561 -> 572 -0.10098
562 -> 573 -0.17937
563 -> 579 -0.11068

Excited State 109: Singlet-A 3.8632 eV 320.94 nm f=0.0152 <S**2>=0.000
558 -> 572 0.16446
562 -> 573 0.61019
562 -> 577 0.10935

Excited State 110: Singlet-A 3.8744 eV 320.00 nm f=0.0008 <S**2>=0.000

563 -> 576 -0.10679

563 -> 581 0.56182

564 -> 582 -0.30537

564 -> 583 0.18153

Excited State 111: Singlet-A 3.9069 eV 317.34 nm f=0.0105 <S**2>=0.000

555 -> 571 0.54941

556 -> 569 0.16144

558 -> 571 -0.34634

563 -> 582 0.10078

Excited State 112: Singlet-A 3.9126 eV 316.88 nm f=0.0016 <S**2>=0.000

555 -> 571 -0.10279

563 -> 582 0.54839

563 -> 583 -0.32615

564 -> 581 -0.17007

Excited State 113: Singlet-A 3.9332 eV 315.22 nm f=0.0042 <S**2>=0.000

554 -> 569 0.29475

556 -> 571 0.60314

559 -> 571 -0.11888

Excited State 114: Singlet-A 3.9553 eV 313.46 nm f=0.0004 <S**2>=0.000

557 -> 572 0.11264

557 -> 573 -0.11419

562 -> 574 0.50755

562 -> 575 -0.36058

562 -> 576 0.12568

562 -> 578 0.16225

Excited State 115: Singlet-A 3.9591 eV 313.16 nm f=0.0109 <S**2>=0.000

555 -> 572 0.54891

556 -> 570 -0.15067

558 -> 572 -0.35158

Excited State 116: Singlet-A 3.9685 eV 312.42 nm f=0.0002 <S**2>=0.000
552 -> 565 0.48068
554 -> 569 -0.38705
556 -> 571 0.18854
556 -> 572 0.18763

Excited State 117: Singlet-A 3.9692 eV 312.36 nm f=0.0009 <S**2>=0.000
552 -> 565 0.48705
554 -> 569 0.36927
556 -> 571 -0.17319
556 -> 572 -0.19814

Excited State 118: Singlet-A 3.9729 eV 312.08 nm f=0.0001 <S**2>=0.000
554 -> 569 -0.14335
563 -> 582 0.27826
563 -> 583 0.47129
564 -> 584 -0.35110

Excited State 119: Singlet-A 3.9751 eV 311.91 nm f=0.0055 <S**2>=0.000
562 -> 575 0.28579
562 -> 576 0.52101
562 -> 577 0.23196

Excited State 120: Singlet-A 3.9847 eV 311.15 nm f=0.0057 <S**2>=0.000
554 -> 569 0.27240
554 -> 570 0.15012
556 -> 571 -0.11830
556 -> 572 0.57308
559 -> 572 0.11107

Excited State 121: Singlet-A 3.9906 eV 310.69 nm f=0.0009 <S**2>=0.000
563 -> 584 0.60463
564 -> 582 -0.14462
564 -> 583 -0.24932

Excited State 122: Singlet-A 3.9976 eV 310.15 nm f=0.0009 <S**2>=0.000

560 -> 573 -0.11750
562 -> 574 0.33103
562 -> 575 0.44614
562 -> 576 -0.25525
562 -> 578 0.11243
562 -> 579 -0.15005

Excited State 123: Singlet-A 4.0142 eV 308.86 nm f=0.0118 <S**2>=0.000
560 -> 573 0.58424
560 -> 577 0.11224
562 -> 574 0.10148
562 -> 575 0.11106
563 -> 585 0.10731

Excited State 124: Singlet-A 4.0163 eV 308.70 nm f=0.0002 <S**2>=0.000
552 -> 566 0.68305

Excited State 125: Singlet-A 4.0317 eV 307.52 nm f=0.0004 <S**2>=0.000
549 -> 565 -0.12665
550 -> 565 -0.11313
552 -> 567 0.66043

Excited State 126: Singlet-A 4.0399 eV 306.90 nm f=0.0096 <S**2>=0.000
553 -> 569 0.21618
554 -> 571 -0.17764
561 -> 573 -0.11686
563 -> 585 -0.14484
563 -> 586 0.16110
564 -> 585 0.39814
564 -> 586 0.21631
564 -> 591 0.12586
564 -> 593 -0.11939

Excited State 127: Singlet-A 4.0447 eV 306.54 nm f=0.0004 <S**2>=0.000
553 -> 572 0.14289
554 -> 570 0.65624

556 -> 572 -0.15918

Excited State 128: Singlet-A 4.0630 eV 305.15 nm f=0.0144 <S**2>=0.000
539 -> 565 0.10404
549 -> 565 0.10413
550 -> 565 0.10746
551 -> 565 0.12741
552 -> 568 -0.12272
553 -> 569 0.46052
554 -> 571 -0.32235
564 -> 585 -0.15155

Excited State 129: Singlet-A 4.0658 eV 304.94 nm f=0.0010 <S**2>=0.000
541 -> 566 -0.12443
542 -> 566 0.21701
543 -> 566 0.15176
546 -> 566 0.12896
549 -> 566 -0.12007
551 -> 565 -0.11073
552 -> 568 0.49686
553 -> 569 0.12194

Excited State 130: Singlet-A 4.0697 eV 304.65 nm f=0.0016 <S**2>=0.000
541 -> 566 0.16826
542 -> 566 -0.23481
542 -> 568 0.12030
543 -> 566 -0.19974
546 -> 566 -0.13947
548 -> 566 0.11262
549 -> 565 0.10244
551 -> 565 0.14126
552 -> 568 0.42544

Excited State 131: Singlet-A 4.0706 eV 304.58 nm f=0.0128 <S**2>=0.000
539 -> 565 0.13897
540 -> 565 0.11099

541 -> 566 -0.13848
542 -> 566 0.20431
543 -> 565 -0.13469
543 -> 566 0.12598
546 -> 566 0.12687
549 -> 565 0.19839
550 -> 565 0.21293
551 -> 565 0.24639
552 -> 567 0.10108
553 -> 569 -0.20236
554 -> 571 0.13749
564 -> 585 0.10484

Excited State 132: Singlet-A 4.0767 eV 304.13 nm f=0.0103 <S**2>=0.000
551 -> 565 -0.26897
559 -> 573 0.13919
560 -> 573 -0.17890
561 -> 575 0.15252
563 -> 585 0.21141
563 -> 586 0.18945
564 -> 585 -0.16701
564 -> 586 0.35010

Excited State 133: Singlet-A 4.0790 eV 303.96 nm f=0.0026 <S**2>=0.000
539 -> 565 -0.25186
540 -> 565 -0.17205
549 -> 565 -0.10206
551 -> 565 0.50927
564 -> 586 0.13327

Excited State 134: Singlet-A 4.0903 eV 303.12 nm f=0.0040 <S**2>=0.000
557 -> 577 -0.10329
561 -> 573 -0.10739
562 -> 574 -0.24926
562 -> 577 -0.11889
562 -> 578 0.47074

562 -> 579 -0.28032
562 -> 582 -0.12968

Excited State 135: Singlet-A 4.0916 eV 303.02 nm f=0.0019 <S**2>=0.000
558 -> 576 0.10339
559 -> 574 -0.15846
559 -> 575 0.13469
561 -> 573 0.51540
564 -> 589 -0.13211

Excited State 136: Singlet-A 4.0991 eV 302.47 nm f=0.0010 <S**2>=0.000
541 -> 568 0.18795
542 -> 566 0.19744
542 -> 568 0.34147
543 -> 566 -0.11621
543 -> 568 -0.31236
546 -> 568 -0.17037
547 -> 568 -0.11826
548 -> 568 0.20753
552 -> 568 -0.10216
561 -> 573 0.13373

Excited State 137: Singlet-A 4.1097 eV 301.68 nm f=0.0006 <S**2>=0.000
538 -> 567 -0.17868
539 -> 565 -0.20984
549 -> 565 0.19560
549 -> 567 -0.15029
550 -> 565 0.32641
550 -> 567 -0.14266
551 -> 565 -0.12019
551 -> 567 0.13457
552 -> 567 0.15678
560 -> 574 -0.18742
560 -> 575 0.13239

Excited State 138: Singlet-A 4.1111 eV 301.58 nm f=0.0125 <S**2>=0.000

550 -> 565 0.13417
558 -> 573 0.10898
560 -> 574 0.40202
560 -> 575 -0.29886
560 -> 578 0.12740
564 -> 585 -0.13052
564 -> 593 0.11078

Excited State 139: Singlet-A 4.1254 eV 300.54 nm f=0.0003 <S**2>=0.000
550 -> 566 0.12213
551 -> 566 -0.23469
559 -> 573 0.14831
560 -> 575 -0.13319
560 -> 576 -0.24041
560 -> 577 -0.10678
561 -> 574 -0.22754
562 -> 578 0.13116
562 -> 579 0.35628

Excited State 140: Singlet-A 4.1266 eV 300.45 nm f=0.0020 <S**2>=0.000
550 -> 566 -0.15630
551 -> 566 0.49470
562 -> 578 0.16476
562 -> 579 0.29011

Excited State 141: Singlet-A 4.1269 eV 300.43 nm f=0.0066 <S**2>=0.000
538 -> 565 0.12782
538 -> 567 -0.14022
539 -> 567 0.10091
551 -> 566 -0.15175
559 -> 573 -0.20228
561 -> 574 0.24160
561 -> 575 -0.10810
562 -> 578 0.22665
562 -> 579 0.28246
564 -> 586 0.10032

Excited State 142: Singlet-A 4.1313 eV 300.11 nm f=0.0054 <S**2>=0.000

538 -> 565 0.10105
538 -> 567 -0.10860
553 -> 570 0.39242
554 -> 572 0.31260
562 -> 576 0.12729
562 -> 577 -0.26394
562 -> 581 0.14057

Excited State 143: Singlet-A 4.1332 eV 299.97 nm f=0.0033 <S**2>=0.000

538 -> 565 0.19865
538 -> 567 -0.19237
539 -> 565 0.12288
539 -> 567 0.16185
540 -> 565 0.11010
549 -> 567 -0.13453
550 -> 565 -0.20459
550 -> 566 -0.10871
550 -> 567 -0.10599
551 -> 565 0.11003
551 -> 566 0.23847
551 -> 567 -0.18190
561 -> 574 -0.12050
562 -> 577 0.14143

Excited State 144: Singlet-A 4.1370 eV 299.70 nm f=0.0198 <S**2>=0.000

553 -> 570 0.31692
554 -> 572 0.23252
562 -> 573 -0.11365
562 -> 576 -0.19255
562 -> 577 0.42143
562 -> 578 0.11369
562 -> 581 -0.21912

Excited State 145: Singlet-A 4.1451 eV 299.11 nm f=0.0007 <S**2>=0.000

539 -> 565 0.14044
550 -> 565 -0.16571
550 -> 567 -0.17680
551 -> 567 0.59543

Excited State 146: Singlet-A 4.1496 eV 298.78 nm f=0.0031 <S**2>=0.000
550 -> 566 0.11223
559 -> 575 0.12357
560 -> 574 0.17817
560 -> 576 0.29822
560 -> 577 0.11963
561 -> 573 -0.15016
561 -> 574 -0.22633
561 -> 575 -0.10102
561 -> 576 -0.19116
562 -> 578 0.10798
564 -> 591 0.10663
564 -> 592 0.12574
564 -> 593 -0.17235

Excited State 147: Singlet-A 4.1527 eV 298.57 nm f=0.0102 <S**2>=0.000
549 -> 566 0.13428
550 -> 566 -0.24000
551 -> 566 -0.14484
559 -> 573 0.13830
560 -> 575 0.26582
560 -> 576 0.24634
560 -> 577 0.10077
561 -> 575 0.24193
562 -> 578 0.13079
562 -> 579 0.10092

Excited State 148: Singlet-A 4.1534 eV 298.51 nm f=0.0002 <S**2>=0.000
549 -> 566 -0.19943
550 -> 566 0.37312
551 -> 566 0.19058

551 -> 568 0.13709
552 -> 568 -0.11533
560 -> 575 0.22211
561 -> 576 0.17845
562 -> 580 0.11210
564 -> 593 0.11447

Excited State 149: Singlet-A 4.1581 eV 298.17 nm f=0.0380 <S**2>=0.000
550 -> 566 0.11693
558 -> 574 0.13930
559 -> 576 -0.20336
560 -> 575 -0.12673
561 -> 574 0.29187
561 -> 575 0.28885
561 -> 576 -0.21381
563 -> 586 -0.12589
563 -> 591 -0.10556
563 -> 592 -0.11811
563 -> 593 0.14737

Excited State 150: Singlet-A 4.1611 eV 297.96 nm f=0.0052 <S**2>=0.000
560 -> 574 -0.29559
560 -> 575 -0.28122
560 -> 576 0.30126
560 -> 577 0.12399
560 -> 579 0.10906
561 -> 573 0.13652
561 -> 574 -0.14573
562 -> 577 -0.11199
562 -> 580 -0.18873
563 -> 586 0.10596
564 -> 593 0.13112

Excited State 151: Singlet-A 4.1748 eV 296.98 nm f=0.0012 <S**2>=0.000
560 -> 574 -0.10127
560 -> 575 -0.19937

562 -> 580 0.61102

Excited State 152: Singlet-A 4.1801 eV 296.61 nm f=0.0028 <S**2>=0.000
538 -> 567 0.17245
549 -> 567 -0.12449
549 -> 568 -0.14341
550 -> 566 -0.11928
550 -> 567 -0.24349
550 -> 568 0.22743
551 -> 566 -0.10265
551 -> 567 -0.10481
551 -> 568 0.42803

Excited State 153: Singlet-A 4.1822 eV 296.46 nm f=0.0093 <S**2>=0.000
538 -> 567 -0.13144
550 -> 567 0.17914
550 -> 568 0.15924
551 -> 567 0.12652
551 -> 568 0.28595
553 -> 569 0.10454
554 -> 571 0.12057
559 -> 575 0.10164
561 -> 576 -0.28599
562 -> 580 0.12322
563 -> 586 0.13017
564 -> 593 0.13077

Excited State 154: Singlet-A 4.1829 eV 296.41 nm f=0.0027 <S**2>=0.000
538 -> 565 0.10063
538 -> 567 -0.21514
549 -> 567 0.15055
550 -> 567 0.30082
551 -> 567 0.17263
551 -> 568 0.14735
553 -> 569 -0.10628
554 -> 571 -0.14432

561 -> 576 0.24386
563 -> 586 -0.11662
564 -> 593 -0.12450

Excited State 155: Singlet-A 4.1856 eV 296.21 nm f=0.0003 <S**2>=0.000
559 -> 577 -0.12734
561 -> 574 -0.17008
561 -> 578 0.13407
563 -> 585 -0.15125
563 -> 591 -0.21794
563 -> 592 -0.19156
563 -> 593 0.28329
564 -> 585 -0.12817
564 -> 586 0.22042
564 -> 588 -0.22263

Excited State 156: Singlet-A 4.1934 eV 295.66 nm f=0.0060 <S**2>=0.000
553 -> 569 0.31230
554 -> 571 0.44542
559 -> 574 -0.10351
561 -> 576 0.10081
561 -> 577 -0.13284
563 -> 588 0.14841
564 -> 589 0.18305
564 -> 593 -0.10862

Excited State 157: Singlet-A 4.1983 eV 295.32 nm f=0.0187 <S**2>=0.000
553 -> 569 0.18614
554 -> 571 0.27275
561 -> 573 -0.10063
561 -> 575 -0.14249
561 -> 576 0.11171
561 -> 577 0.15738
563 -> 588 -0.19977
564 -> 585 -0.10237
564 -> 587 0.15960

564 -> 588 0.22715
564 -> 589 -0.22735

Excited State 158: Singlet-A 4.2021 eV 295.05 nm f=0.0021 <S**2>=0.000
541 -> 566 -0.11791
541 -> 568 -0.11290
542 -> 568 -0.13667
549 -> 568 -0.24807
550 -> 568 0.41100
551 -> 568 -0.39449

Excited State 159: Singlet-A 4.2045 eV 294.89 nm f=0.0338 <S**2>=0.000
559 -> 578 0.10263
561 -> 575 -0.25311
561 -> 578 -0.18549
563 -> 588 0.11239
563 -> 589 0.24214
564 -> 586 0.14426
564 -> 587 0.11292
564 -> 588 0.18870
564 -> 589 0.32144

Excited State 160: Singlet-A 4.2394 eV 292.45 nm f=0.0008 <S**2>=0.000
559 -> 574 0.11325
560 -> 578 -0.10429
562 -> 577 0.22181
562 -> 581 0.59582

Excited State 161: Singlet-A 4.2471 eV 291.93 nm f=0.0046 <S**2>=0.000
537 -> 565 -0.10573
539 -> 565 0.19932
540 -> 565 0.15189
543 -> 565 0.12510
544 -> 565 -0.16908
545 -> 565 0.11149
546 -> 565 -0.18232

548 -> 565 0.17495
549 -> 565 -0.32745
550 -> 565 0.34899
550 -> 567 0.12177

Excited State 162: Singlet-A 4.2485 eV 291.83 nm f=0.0038 <S**2>=0.000
553 -> 570 0.11409
554 -> 572 -0.15692
559 -> 573 0.17556
559 -> 574 0.25707
560 -> 578 0.23693
560 -> 579 -0.12758
561 -> 573 0.10634
561 -> 577 0.26272
561 -> 581 0.11748
563 -> 588 0.12573
564 -> 588 -0.10527
564 -> 589 0.16779

Excited State 163: Singlet-A 4.2559 eV 291.33 nm f=0.0015 <S**2>=0.000
553 -> 570 -0.31336
554 -> 572 0.36675
560 -> 574 -0.19147
560 -> 578 0.32616
560 -> 579 -0.16115
561 -> 577 -0.10492

Excited State 164: Singlet-A 4.2597 eV 291.06 nm f=0.0097 <S**2>=0.000
553 -> 570 -0.25660
554 -> 572 0.34029
559 -> 573 0.25624
559 -> 574 0.12818
560 -> 574 0.15505
560 -> 578 -0.22272
560 -> 579 0.10910
561 -> 577 0.13816

562 -> 581 -0.12376

Excited State 165: Singlet-A 4.2631 eV 290.83 nm f=0.0050 <S**2>=0.000
538 -> 567 0.14095
539 -> 565 0.12660
543 -> 565 0.19396
545 -> 565 0.17820
546 -> 565 -0.15369
547 -> 565 0.12780
548 -> 565 0.18192
549 -> 565 0.42674
550 -> 565 -0.17723
550 -> 567 0.12367

Excited State 166: Singlet-A 4.2655 eV 290.67 nm f=0.0014 <S**2>=0.000
554 -> 572 -0.12161
559 -> 573 0.41022
559 -> 574 -0.19745
561 -> 574 0.17007
561 -> 575 -0.16473
561 -> 577 -0.14378
561 -> 578 -0.15658
561 -> 579 -0.10242
564 -> 588 -0.15161

Excited State 167: Singlet-A 4.2734 eV 290.13 nm f=0.0012 <S**2>=0.000
561 -> 578 0.10032
561 -> 579 0.11104
563 -> 592 0.10745
564 -> 587 0.54505
564 -> 588 -0.19858

Excited State 168: Singlet-A 4.2740 eV 290.09 nm f=0.0044 <S**2>=0.000
534 -> 566 -0.21016
535 -> 566 0.10811
541 -> 566 0.26404

542 -> 566 -0.21205
546 -> 566 0.26236
548 -> 566 -0.23038
550 -> 566 -0.25545
550 -> 568 0.15475

Excited State 169: Singlet-A 4.2831 eV 289.47 nm f=0.1091 <S**2>=0.000
553 -> 571 -0.25940
559 -> 576 0.13164
559 -> 577 0.14397
559 -> 580 0.13461
560 -> 577 -0.10702
560 -> 578 -0.10221
560 -> 579 -0.11183
561 -> 579 0.35879
562 -> 582 0.20613
562 -> 583 -0.13188
564 -> 586 0.15458

Excited State 170: Singlet-A 4.2837 eV 289.44 nm f=0.0142 <S**2>=0.000
553 -> 571 -0.30262
558 -> 580 -0.10214
559 -> 578 0.10550
560 -> 578 0.23204
560 -> 579 0.40431
561 -> 580 0.22576
564 -> 589 -0.10431

Excited State 171: Singlet-A 4.2847 eV 289.36 nm f=0.0045 <S**2>=0.000
553 -> 571 0.46457
560 -> 577 -0.21917
560 -> 579 0.18253
562 -> 582 0.25126
562 -> 583 -0.14825

Excited State 172: Singlet-A 4.2883 eV 289.12 nm f=0.0018 <S**2>=0.000

538 -> 565 0.13514
543 -> 565 -0.11900
544 -> 565 0.19390
545 -> 565 0.34394
545 -> 567 0.14606
546 -> 565 0.30433
547 -> 565 0.18331
547 -> 567 0.15721
548 -> 565 0.10326
548 -> 567 0.15526
550 -> 567 -0.13208

Excited State 173: Singlet-A 4.2902 eV 288.99 nm f=0.0762 <S**2>=0.000
553 -> 571 -0.24754
559 -> 576 -0.12330
559 -> 577 -0.12302
560 -> 577 -0.14977
561 -> 579 -0.26966
562 -> 582 0.34057
562 -> 583 -0.19622
564 -> 586 -0.10145
564 -> 587 0.14821

Excited State 174: Singlet-A 4.2928 eV 288.82 nm f=0.0136 <S**2>=0.000
553 -> 571 0.12098
559 -> 576 0.10135
559 -> 577 -0.16368
560 -> 577 0.22181
561 -> 574 0.12893
561 -> 577 -0.13712
561 -> 578 0.33487
562 -> 582 0.21495
562 -> 583 -0.13082
564 -> 588 0.21735

Excited State 175: Singlet-A 4.2980 eV 288.47 nm f=0.0028 <S**2>=0.000

559 -> 574 0.11656
559 -> 575 -0.31952
560 -> 578 -0.12743
560 -> 579 -0.28780
561 -> 577 -0.14748
561 -> 580 0.32872

Excited State 176: Singlet-A 4.3024 eV 288.18 nm f=0.0026 <S**2>=0.000
541 -> 568 0.12158
542 -> 568 0.16731
543 -> 566 0.10638
546 -> 566 0.10221
548 -> 566 -0.10452
549 -> 566 0.48962
550 -> 566 0.26502
550 -> 568 0.14155

Excited State 177: Singlet-A 4.3041 eV 288.06 nm f=0.0056 <S**2>=0.000
538 -> 565 -0.12847
538 -> 567 0.16358
543 -> 567 -0.15565
544 -> 567 0.16073
546 -> 567 0.22422
547 -> 565 0.10429
547 -> 567 -0.11488
548 -> 567 -0.16910
550 -> 567 0.16789
560 -> 576 0.10979
560 -> 577 -0.20831
560 -> 581 0.11913
561 -> 578 0.14205
562 -> 582 -0.10642

Excited State 178: Singlet-A 4.3061 eV 287.93 nm f=0.0015 <S**2>=0.000
538 -> 567 0.12363
543 -> 567 -0.11449

544 -> 567 0.11936
546 -> 567 0.16853
548 -> 567 -0.12746
550 -> 567 0.14025
559 -> 573 -0.13971
559 -> 577 0.11208
560 -> 576 -0.14595
560 -> 577 0.28840
560 -> 581 -0.16172
561 -> 577 0.11928
561 -> 578 -0.19367
562 -> 582 0.13593

Excited State 179: Singlet-A 4.3134 eV 287.44 nm f=0.0054 <S**2>=0.000
536 -> 568 -0.10687
542 -> 566 0.10125
548 -> 568 -0.10978
549 -> 566 -0.11599
550 -> 568 0.11557
559 -> 574 0.33026
559 -> 578 0.13573
559 -> 579 -0.19731
561 -> 577 -0.19394
561 -> 578 -0.15165
561 -> 580 -0.13658
561 -> 581 0.16691

Excited State 180: Singlet-A 4.3147 eV 287.35 nm f=0.0011 <S**2>=0.000
536 -> 568 -0.20752
541 -> 568 0.15114
542 -> 566 0.17813
542 -> 568 0.16920
543 -> 568 0.11075
544 -> 566 0.11438
546 -> 568 0.16726
548 -> 568 -0.22187

549 -> 566 -0.21200
550 -> 568 0.22616
559 -> 574 -0.18165
559 -> 579 0.10002

Excited State 181: Singlet-A 4.3171 eV 287.19 nm f=0.0001 <S**2>=0.000
545 -> 567 0.15915
547 -> 567 -0.16715
548 -> 567 -0.14206
549 -> 567 0.50818
550 -> 567 -0.27888

Excited State 182: Singlet-A 4.3243 eV 286.72 nm f=0.0037 <S**2>=0.000
559 -> 575 0.32257
559 -> 578 0.19783
559 -> 579 0.21545
560 -> 580 -0.16774
561 -> 576 0.12913
561 -> 580 0.19819
561 -> 583 -0.13017
562 -> 582 -0.17119
562 -> 583 -0.24738

Excited State 183: Singlet-A 4.3285 eV 286.43 nm f=0.0012 <S**2>=0.000
559 -> 576 -0.31970
559 -> 578 0.10886
560 -> 580 0.44907
561 -> 578 -0.10570
562 -> 583 -0.14196

Excited State 184: Singlet-A 4.3345 eV 286.04 nm f=0.0018 <S**2>=0.000
537 -> 565 -0.13212
543 -> 567 0.20493
544 -> 567 -0.13106
545 -> 565 -0.16860
545 -> 567 0.38876

546 -> 567 -0.17619
547 -> 565 0.10173
547 -> 567 -0.27398
548 -> 567 -0.10176
549 -> 567 -0.21613

Excited State 185: Singlet-A 4.3367 eV 285.90 nm f=0.0033 <S**2>=0.000
559 -> 575 0.11731
560 -> 580 0.12123
563 -> 585 -0.34248
563 -> 586 0.35124
563 -> 587 -0.10945
564 -> 585 -0.28096
564 -> 586 -0.17409
564 -> 591 0.11260

Excited State 186: Singlet-A 4.3423 eV 285.53 nm f=0.0046 <S**2>=0.000
537 -> 565 -0.10638
553 -> 572 0.10630
559 -> 575 -0.13177
562 -> 582 -0.13203
562 -> 583 -0.20449
563 -> 585 -0.18950
563 -> 587 0.37231
564 -> 590 0.15253
564 -> 591 -0.15409
564 -> 592 0.15089
564 -> 594 0.10921

Excited State 187: Singlet-A 4.3443 eV 285.39 nm f=0.0006 <S**2>=0.000
537 -> 565 -0.11296
553 -> 572 0.12426
559 -> 575 0.14093
559 -> 576 0.27114
559 -> 580 -0.15573
560 -> 580 0.29848

561 -> 575 0.15947
561 -> 579 -0.18434
562 -> 582 0.11488
562 -> 583 0.23401
562 -> 584 -0.10801
563 -> 586 -0.10264

Excited State 188: Singlet-A 4.3456 eV 285.31 nm f=0.0003 <S**2>=0.000
553 -> 572 0.64621
554 -> 570 -0.13591

Excited State 189: Singlet-A 4.3472 eV 285.21 nm f=0.0030 <S**2>=0.000
559 -> 576 -0.18946
560 -> 580 -0.15251
561 -> 580 0.11807
562 -> 582 0.24639
562 -> 583 0.39055
563 -> 587 0.24470
564 -> 591 -0.10473

Excited State 190: Singlet-A 4.3497 eV 285.04 nm f=0.0129 <S**2>=0.000
535 -> 565 -0.28207
536 -> 565 -0.14540
537 -> 565 0.38351
537 -> 567 0.11427
538 -> 565 0.14102
539 -> 565 -0.10300
540 -> 565 0.11486
560 -> 580 0.16118
563 -> 587 0.13590

Excited State 191: Singlet-A 4.3526 eV 284.85 nm f=0.0016 <S**2>=0.000
541 -> 566 0.12774
542 -> 568 -0.22623
543 -> 568 -0.12511
544 -> 566 0.17932

548 -> 568 0.11013
549 -> 566 0.12821
549 -> 568 0.44161
550 -> 568 0.21875

Excited State 192: Singlet-A 4.3585 eV 284.47 nm f=0.0183 <S**2>=0.000
559 -> 576 0.14375
563 -> 585 0.25685
563 -> 586 0.31698
563 -> 587 0.14606
563 -> 592 -0.15551
563 -> 593 0.10378
564 -> 586 -0.18211
564 -> 590 -0.28930

Excited State 193: Singlet-A 4.3602 eV 284.35 nm f=0.0022 <S**2>=0.000
534 -> 566 -0.14258
541 -> 566 0.17584
541 -> 568 -0.12730
542 -> 566 0.21295
543 -> 566 0.14572
544 -> 566 0.33077
544 -> 568 -0.15803
549 -> 566 0.14053
549 -> 568 -0.32064
550 -> 568 -0.13696

Excited State 194: Singlet-A 4.3672 eV 283.90 nm f=0.0044 <S**2>=0.000
557 -> 573 -0.31122
562 -> 575 0.13883
562 -> 584 0.55700

Excited State 195: Singlet-A 4.3700 eV 283.71 nm f=0.0025 <S**2>=0.000
534 -> 566 0.29186
541 -> 566 -0.11304
541 -> 568 0.10674

542 -> 566 -0.17797
543 -> 566 0.28741
543 -> 568 -0.13036
544 -> 566 0.30836
544 -> 568 -0.14148
562 -> 584 -0.12520

Excited State 196: Singlet-A 4.3739 eV 283.46 nm f=0.0018 <S**2>=0.000
557 -> 573 0.48829
560 -> 580 0.11312
562 -> 578 0.12653
562 -> 584 0.31216

Excited State 197: Singlet-A 4.3754 eV 283.36 nm f=0.0024 <S**2>=0.000
559 -> 581 0.11522
560 -> 581 -0.15471
561 -> 582 -0.11772
563 -> 585 0.16268
563 -> 586 0.11451
563 -> 593 0.21865
564 -> 586 -0.15530
564 -> 588 0.11293
564 -> 590 0.43848

Excited State 198: Singlet-A 4.3805 eV 283.04 nm f=0.0000 <S**2>=0.000
543 -> 568 0.17127
544 -> 566 -0.13521
544 -> 568 -0.10875
545 -> 568 -0.10268
546 -> 566 0.14284
546 -> 568 0.40146
547 -> 568 -0.32899
548 -> 568 0.28257
549 -> 568 -0.10409

Excited State 199: Singlet-A 4.3889 eV 282.49 nm f=0.0125 <S**2>=0.000

| | |
|---|---|
| 538 -> 565 | 0.12313 |
| 558 -> 573 | 0.33794 |
| 558 -> 581 | 0.10216 |
| 559 -> 574 | -0.15280 |
| 559 -> 582 | -0.13233 |
| 560 -> 581 | 0.12287 |
| 561 -> 576 | -0.17204 |
| 561 -> 581 | 0.29205 |
| 564 -> 590 | 0.12543 |

Excited State 200: Singlet-A 4.3907 eV 282.38 nm f=0.0079 <S**2>=0.000

| | |
|---|---|
| 535 -> 565 | 0.22861 |
| 535 -> 567 | -0.13193 |
| 537 -> 567 | -0.16671 |
| 538 -> 565 | 0.34058 |
| 538 -> 567 | 0.13915 |
| 539 -> 565 | -0.13204 |
| 539 -> 567 | -0.15286 |
| 540 -> 567 | -0.10379 |
| 560 -> 581 | -0.19427 |
| 561 -> 581 | -0.13611 |
| 564 -> 590 | -0.11529 |

**Table S8.** Standard orientation of the optimized geometry for the open-ring isomer(OF1) of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | -0.18024 | -2.14154 | -0.21421 |
| N | -4.46048 | -2.55754 | 0.14895 |
| C | -3.41173 | -1.94397 | -0.51338 |
| C | -3.9597 | -1.22071 | -1.65747 |
| C | -5.36079 | -1.44221 | -1.66196 |
| C | -5.79125 | -2.34473 | -0.47736 |
| C | -6.74106 | -1.60105 | 0.436099 |
| C | -8.02737 | -1.95941 | 0.589833 |
| C | -8.588 | -3.16357 | -0.05481 |
| C | -7.65047 | -3.9928 | -0.83741 |
| C | -6.36323 | -3.64517 | -1.00486 |
| O | -9.79383 | -3.47519 | 0.072178 |
| C | -3.3761 | -0.46763 | -2.68178 |
| C | -4.20336 | 0.058606 | -3.68426 |
| C | -5.58839 | -0.1589 | -3.67762 |
| C | -6.17903 | -0.91927 | -2.65482 |
| C | -3.96517 | -3.40561 | 1.136753 |
| C | -2.58365 | -3.27231 | 1.05803 |
| N | -2.25309 | -2.34826 | 0.035624 |
| C | -4.83165 | -4.2572 | 1.979145 |
| C | -1.46792 | -3.96515 | 1.676591 |
| C | -1.59301 | -4.89171 | 2.72688 |
| C | -0.48035 | -5.61383 | 3.159835 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.753347 | -5.42082 | 2.52689 | C | 5.972867 | -3.92338 | 0.300919 |
| C | 0.885903 | -4.47753 | 1.500448 | C | 7.285289 | -4.12063 | 0.090191 |
| C | -0.20379 | -3.69481 | 1.075824 | C | 8.20734 | -3.00445 | -0.20033 |
| C | -5.65377 | -3.69254 | 2.972049 | C | 7.616381 | -1.65444 | -0.26242 |
| C | -6.48546 | -4.50437 | 3.74991 | C | 6.305202 | -1.43542 | -0.05818 |
| C | -6.50106 | -5.8897 | 3.551965 | O | 9.430346 | -3.19758 | -0.39113 |
| C | -5.67882 | -6.46251 | 2.573772 | C | 2.70784 | -1.64486 | 2.865197 |
| C | -4.85159 | -5.65319 | 1.790518 | C | 3.412547 | -1.64436 | 4.075935 |
| N | -4.00137 | 2.946959 | -0.16512 | C | 4.783746 | -1.92858 | 4.121661 |
| C | -3.02761 | 2.216077 | 0.491191 | C | 5.485258 | -2.2202 | 2.941743 |
| C | -3.65346 | 1.545001 | 1.627767 | C | 3.65767 | -3.00433 | -1.68133 |
| C | -5.02099 | 1.92041 | 1.634309 | C | 2.271775 | -2.86508 | -1.66809 |
| C | -5.34998 | 2.87072 | 0.455139 | N | 1.873537 | -2.28671 | -0.44094 |
| C | -5.78684 | 4.220852 | 0.98633 | C | 4.57849 | -3.6249 | -2.65358 |
| C | -7.03007 | 4.700543 | 0.813554 | C | 1.178637 | -3.30738 | -2.52212 |
| C | -8.04385 | 3.976381 | 0.021098 | C | 1.331228 | -3.82991 | -3.81791 |
| C | -7.60692 | 2.724084 | -0.62709 | C | 0.224741 | -4.32827 | -4.50899 |
| C | -6.3655 | 2.233793 | -0.46841 | C | -1.03565 | -4.31261 | -3.89988 |
| O | -9.2098 | 4.41254 | -0.11029 | C | -1.19816 | -3.76552 | -2.62028 |
| C | -3.15858 | 0.71644 | 2.639935 | C | -0.11165 | -3.22122 | -1.91484 |
| C | -4.03974 | 0.274479 | 3.636962 | C | 5.651825 | -2.90308 | -3.20874 |
| C | -5.39077 | 0.648528 | 3.635821 | C | 6.540142 | -3.52179 | -4.094 |
| C | -5.89273 | 1.481418 | 2.622198 | C | 6.364552 | -4.8647 | -4.44635 |
| C | -3.4189 | 3.737601 | -1.15262 | C | 5.293774 | -5.58899 | -3.90773 |
| C | -2.06144 | 3.450498 | -1.07863 | C | 4.410166 | -4.97731 | -3.01495 |
| N | -1.83325 | 2.494998 | -0.05882 | N | 4.563354 | 1.764254 | 0.840705 |
| C | -4.18596 | 4.679142 | -1.99541 | C | 3.514047 | 1.671762 | -0.07168 |
| C | -0.87801 | 3.993222 | -1.71747 | C | 3.834066 | 1.430083 | -1.45388 |
| C | -0.8969 | 4.912293 | -2.78148 | C | 2.938454 | 0.777933 | -2.33135 |
| C | 0.297138 | 5.452446 | -3.25996 | C | 3.340139 | 0.362647 | -3.58919 |
| C | 1.51028 | 5.080454 | -2.66728 | C | 4.665149 | 0.586588 | -4.02625 |
| C | 1.530739 | 4.148548 | -1.62348 | C | 5.554088 | 1.264065 | -3.21046 |
| C | 0.350098 | 3.5598 | -1.14205 | C | 4.051867 | 2.234765 | 1.990602 |
| C | -5.06547 | 4.207908 | -2.98796 | C | 2.62114 | 2.383985 | 1.822468 |
| C | -5.80018 | 5.106876 | -3.76753 | N | 2.299158 | 1.953665 | 0.541675 |
| C | -5.66044 | 6.485595 | -3.57183 | C | 4.940065 | 2.517135 | 3.131332 |
| C | -4.7797 | 6.964553 | -2.59418 | C | 1.561981 | 2.951025 | 2.597745 |
| C | -4.04893 | 6.06877 | -1.80906 | C | 1.666899 | 3.391853 | 3.940089 |
| Cl | -0.23367 | 0.150683 | -1.64771 | C | 0.616779 | 4.078696 | 4.530635 |
| Cl | -0.07315 | -0.1901 | 1.645214 | C | -0.54994 | 4.349404 | 3.786322 |
| Ir | 0.199534 | 2.054527 | 0.196971 | C | -0.69014 | 3.872563 | 2.484024 |
| N | 4.078316 | -2.50568 | -0.44468 | C | 0.329979 | 3.114322 | 1.87092 |
| C | 2.980302 | -2.11671 | 0.300106 | C | 5.936577 | 1.584482 | 3.479209 |
| C | 3.402731 | -1.93055 | 1.685458 | C | 6.840813 | 1.85919 | 4.507153 |
| C | 4.78661 | -2.22455 | 1.741956 | C | 6.778288 | 3.076663 | 5.196405 |
| C | 5.350333 | -2.54587 | 0.335962 | C | 5.808487 | 4.021714 | 4.842845 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.898194 | 3.747094 | 3.818223 | H | 1.652437 | -1.41957 | 2.838757 |
| H | -6.32787 | -0.72929 | 0.93335 | H | 2.879501 | -1.42341 | 4.994401 |
| H | -8.70756 | -1.39037 | 1.214485 | H | 5.30645 | -1.92764 | 5.072184 |
| H | -8.05436 | -4.90717 | -1.25803 | H | 6.544715 | -2.45365 | 2.968327 |
| H | -5.67434 | -4.26187 | -1.57455 | H | 2.30956 | -3.8518 | -4.28458 |
| H | -2.31052 | -0.28741 | -2.69191 | H | 0.346769 | -4.73134 | -5.50944 |
| H | -3.75358 | 0.636971 | -4.48439 | H | -1.89649 | -4.71788 | -4.42495 |
| H | -6.20676 | 0.246793 | -4.47154 | H | -2.18709 | -3.75203 | -2.17728 |
| H | -7.24755 | -1.10958 | -2.65113 | H | 5.78326 | -1.85876 | -2.95161 |
| H | -2.55518 | -5.05445 | 3.198656 | H | 7.366804 | -2.95471 | -4.50987 |
| H | -0.57763 | -6.32823 | 3.971163 | H | 7.055113 | -5.34258 | -5.13369 |
| H | 1.618504 | -6.00041 | 2.837295 | H | 5.151919 | -6.6312 | -4.17521 |
| H | 1.854959 | -4.35273 | 1.035008 | H | 3.585361 | -5.54124 | -2.5922 |
| H | -5.62912 | -2.62051 | 3.136676 | H | 1.940913 | 0.548621 | -1.99269 |
| H | -7.11608 | -4.05732 | 4.511643 | H | 2.635756 | -0.16383 | -4.22376 |
| H | -7.14651 | -6.51842 | 4.156668 | H | 4.976736 | 0.255418 | -5.01143 |
| H | -5.68466 | -7.5365 | 2.418609 | H | 6.542883 | 1.507743 | -3.58245 |
| H | -4.21151 | -6.09579 | 1.034374 | H | 2.563457 | 3.184048 | 4.509141 |
| H | -5.04183 | 4.760274 | 1.563791 | H | 0.695513 | 4.412941 | 5.559853 |
| H | -7.3401 | 5.649577 | 1.237064 | H | -1.35545 | 4.919681 | 4.240621 |
| H | -8.33753 | 2.231135 | -1.25935 | H | -1.60785 | 4.071426 | 1.944856 |
| H | -6.04194 | 1.326758 | -0.96868 | H | 5.989097 | 0.648363 | 2.93727 |
| H | -2.12089 | 0.41288 | 2.641667 | H | 7.598289 | 1.126365 | 4.767162 |
| H | -3.65939 | -0.36483 | 4.426532 | H | 7.485435 | 3.291727 | 5.991085 |
| H | -6.0507 | 0.305942 | 4.42607 | H | 5.770052 | 4.97922 | 5.352376 |
| H | -6.93337 | 1.789856 | 2.621707 | H | 4.174606 | 4.500509 | 3.527689 |
| H | -1.83771 | 5.206048 | -3.23204 | C | 5.153828 | 1.772708 | -1.941 |
| H | 0.281526 | 6.161074 | -4.08182 | C | 6.033238 | 2.71129 | -1.27677 |
| H | 2.442667 | 5.510233 | -3.02232 | C | 7.462491 | 2.5441 | -1.35873 |
| H | 2.479838 | 3.864618 | -1.1928 | C | 5.543588 | 3.921068 | -0.66283 |
| H | -5.16083 | 3.139772 | -3.15173 | C | 8.323215 | 3.454189 | -0.81532 |
| H | -6.47611 | 4.732127 | -4.52931 | H | 7.851339 | 1.638741 | -1.81348 |
| H | -6.23081 | 7.181602 | -4.17825 | C | 6.3899 | 4.863791 | -0.15656 |
| H | -4.66495 | 8.032671 | -2.44107 | H | 4.475463 | 4.09831 | -0.65162 |
| H | -3.36415 | 6.438371 | -1.05276 | H | 9.397056 | 3.302986 | -0.82841 |
| H | 5.297214 | -4.75038 | 0.498014 | H | 6.018846 | 5.789849 | 0.267493 |
| H | 7.722793 | -5.11289 | 0.103665 | C | 7.836991 | 4.681008 | -0.18006 |
| H | 8.299915 | -0.84143 | -0.48308 | O | 8.637209 | 5.538298 | 0.299855 |
| H | 5.879058 | -0.43625 | -0.0792 | | | | |

Excited State 1: 3.000-A -0.5851 eV -2118.90 nm f=-0.0000 <S**2>=2.000

433A -> 437A -0.28770

434A -> 437A 0.15211

435A -> 437A 0.60982
433B -> 437B 0.28770
434B -> 437B -0.15211
435B -> 437B -0.60982
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -6024.03416658
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.000-A 0.4485 eV 2764.12 nm f=0.0000 <S**2>=2.000
433A -> 437A -0.13553
436A -> 437A -0.69153
433B -> 437B 0.13553
436B -> 437B 0.69154

Excited State 3: 1.000-A 0.4728 eV 2622.13 nm f=0.0032 <S**2>=0.000
436A -> 437A 0.70264
436B -> 437B 0.70263

Excited State 4: 3.000-A 0.6698 eV 1850.94 nm f=0.0000 <S**2>=2.000
428A -> 437A -0.13673
432A -> 437A 0.11685
433A -> 437A 0.52800
434A -> 437A -0.22210
435A -> 437A 0.35711
436A -> 437A -0.10531
428B -> 437B 0.13673
432B -> 437B -0.11685
433B -> 437B -0.52800
434B -> 437B 0.22210
435B -> 437B -0.35710
436B -> 437B 0.10531

Excited State 5: 1.000-A 0.8450 eV 1467.27 nm f=0.0711 <S**2>=0.000
433A -> 437A 0.30898
434A -> 437A -0.22835
435A -> 437A 0.60545

433B -> 437B 0.30899
434B -> 437B -0.22835
435B -> 437B 0.60545
435A <- 437A -0.15327
435B <- 437B -0.15327

Excited State 6: 3.000-A 0.9738 eV 1273.19 nm f=0.0000 <S**2>=2.000
428A -> 437A -0.12783
429A -> 437A -0.31715
432A -> 437A 0.37937
434A -> 437A 0.46622
428B -> 437B 0.12782
429B -> 437B 0.31715
432B -> 437B -0.37937
434B -> 437B -0.46622

Excited State 7: 1.000-A 1.0328 eV 1200.48 nm f=0.0069 <S**2>=0.000
429A -> 437A -0.12773
432A -> 437A 0.26917
433A -> 437A 0.19772
434A -> 437A 0.59582
435A -> 437A 0.13094
429B -> 437B -0.12773
432B -> 437B 0.26917
433B -> 437B 0.19772
434B -> 437B 0.59583
435B -> 437B 0.13094

Excited State 8: 3.000-A 1.0849 eV 1142.78 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.26015
431A -> 437A -0.16278
432A -> 437A -0.32439
433A -> 437A 0.28875
434A -> 437A 0.44690
429B -> 437B -0.26014
431B -> 437B 0.16278

432B -> 437B 0.32438
433B -> 437B -0.28873
434B -> 437B -0.44689

Excited State 9: 1.000-A 1.1087 eV 1118.25 nm f=0.0104 <S**2>=0.000
429A -> 437A -0.22678
431A -> 437A 0.14432
432A -> 437A 0.44762
433A -> 437A -0.41934
434A -> 437A -0.14591
435A -> 437A 0.16315
429B -> 437B -0.22679
431B -> 437B 0.14432
432B -> 437B 0.44764
433B -> 437B -0.41934
434B -> 437B -0.14592
435B -> 437B 0.16315

Excited State 10: 3.000-A 1.1625 eV 1066.50 nm f=0.0000 <S**2>=2.000
424A -> 437A 0.69278
424B -> 437B -0.69277

Excited State 11: 3.000-A 1.2688 eV 977.21 nm f=0.0000 <S**2>=2.000
428A -> 437A 0.12335
429A -> 437A 0.44209
430A -> 437A -0.18854
431A -> 437A -0.13231
432A -> 437A 0.46017
428B -> 437B -0.12335
429B -> 437B -0.44209
430B -> 437B 0.18853
431B -> 437B 0.13231
432B -> 437B -0.46017

Excited State 12: 1.000-A 1.3018 eV 952.41 nm f=0.0305 <S**2>=0.000
428A -> 437A 0.15113

429A -> 437A 0.38884
430A -> 437A -0.10784
431A -> 437A -0.15464
432A -> 437A 0.45677
433A -> 437A 0.16909
434A -> 437A -0.13090
435A -> 437A -0.20747
428B -> 437B 0.15113
429B -> 437B 0.38885
430B -> 437B -0.10784
431B -> 437B -0.15464
432B -> 437B 0.45677
433B -> 437B 0.16909
434B -> 437B -0.13090
435B -> 437B -0.20747
435A <- 437A 0.10312
435B <- 437B 0.10312

Excited State 13: 3.000-A 1.3526 eV 916.65 nm f=0.0000 <S**2>=2.000
426A -> 437A 0.16880
428A -> 437A 0.20535
429A -> 437A 0.18544
430A -> 437A 0.58202
431A -> 437A 0.17433
432A -> 437A 0.10086
426B -> 437B -0.16879
428B -> 437B -0.20534
429B -> 437B -0.18545
430B -> 437B -0.58195
431B -> 437B -0.17430
432B -> 437B -0.10085

Excited State 14: 1.000-A 1.3596 eV 911.89 nm f=0.0284 <S**2>=0.000
426A -> 437A 0.11501
430A -> 437A 0.55352
431A -> 437A 0.23036

433A -> 437A 0.25425
434A -> 437A -0.11933
435A -> 437A -0.16360
426B -> 437B 0.11503
430B -> 437B 0.55359
431B -> 437B 0.23039
433B -> 437B 0.25426
434B -> 437B -0.11933
435B -> 437B -0.16360

Excited State 15: 1.000-A 1.4024 eV 884.11 nm f=0.0323 <S**2>=0.000
428A -> 437A -0.10951
429A -> 437A 0.50923
430A -> 437A 0.14510
431A -> 437A 0.30738
433A -> 437A -0.21902
434A -> 437A 0.17597
435A -> 437A 0.16650
428B -> 437B -0.10920
429B -> 437B 0.50902
430B -> 437B 0.14515
431B -> 437B 0.30706
433B -> 437B -0.21895
434B -> 437B 0.17591
435B -> 437B 0.16651

Excited State 16: 3.000-A 1.4028 eV 883.81 nm f=0.0000 <S**2>=2.000
428A -> 437A 0.41918
429A -> 437A -0.28512
431A -> 437A -0.44888
428B -> 437B -0.41926
429B -> 437B 0.28549
431B -> 437B 0.44910

Excited State 17: 1.000-A 1.4521 eV 853.83 nm f=0.0262 <S**2>=0.000
430A -> 437A -0.37358

431A -> 437A 0.54054
433A -> 437A 0.18596
435A -> 437A -0.14628
430B -> 437B -0.37359
431B -> 437B 0.54055
433B -> 437B 0.18596
435B -> 437B -0.14628

Excited State 18: 3.000-A 1.4646 eV 846.53 nm f=0.0000 <S**2>=2.000
428A -> 437A 0.45007
430A -> 437A -0.25953
431A -> 437A 0.45663
428B -> 437B -0.45006
430B -> 437B 0.25952
431B -> 437B -0.45661

Excited State 19: 1.000-A 1.5103 eV 820.94 nm f=0.0125 <S**2>=0.000
424A -> 437A -0.28218
428A -> 437A 0.61976
424B -> 437B -0.28219
428B -> 437B 0.61977

Excited State 20: 1.000-A 1.5440 eV 802.99 nm f=0.0182 <S**2>=0.000
424A -> 437A 0.62998
428A -> 437A 0.25170
433A -> 437A -0.11272
435A -> 437A 0.11246
424B -> 437B 0.62999
428B -> 437B 0.25170
433B -> 437B -0.11272
435B -> 437B 0.11246

Excited State 21: 3.000-A 1.5804 eV 784.49 nm f=0.0000 <S**2>=2.000
426A -> 437A 0.59363
427A -> 437A 0.28902
430A -> 437A -0.20809

426B -> 437B -0.59361
427B -> 437B -0.28900
430B -> 437B 0.20808

Excited State 22: 1.000-A 1.6296 eV 760.82 nm f=0.0012 <S**2>=0.000
426A -> 437A 0.60725
427A -> 437A 0.31093
430A -> 437A -0.13048
426B -> 437B 0.60727
427B -> 437B 0.31094
430B -> 437B -0.13049

Excited State 23: 3.000-A 1.8085 eV 685.57 nm f=0.0000 <S**2>=2.000
436A -> 438A -0.54613
436A -> 439A 0.44039
436B -> 438B 0.54620
436B -> 439B -0.44044

Excited State 24: 1.000-A 1.8117 eV 684.34 nm f=0.0000 <S**2>=0.000
436A -> 438A 0.55737
436A -> 439A -0.42788
436B -> 438B 0.55730
436B -> 439B -0.42782

Excited State 25: 3.000-A 1.8154 eV 682.95 nm f=0.0000 <S**2>=2.000
425A -> 437A -0.41439
426A -> 437A -0.24600
427A -> 437A 0.50213
425B -> 437B 0.41439
426B -> 437B 0.24599
427B -> 437B -0.50212

Excited State 26: 1.000-A 1.8576 eV 667.43 nm f=0.0017 <S**2>=0.000
425A -> 437A -0.12606
426A -> 437A -0.32071
427A -> 437A 0.61463

425B -> 437B -0.12607
426B -> 437B -0.32071
427B -> 437B 0.61464

Excited State 27: 3.000-A 1.8701 eV 663.00 nm f=0.0000 <S**2>=2.000
436A -> 438A -0.44155
436A -> 439A -0.54282
436B -> 438B 0.44158
436B -> 439B 0.54285

Excited State 28: 1.000-A 1.8715 eV 662.50 nm f=0.0001 <S**2>=0.000
436A -> 438A 0.42868
436A -> 439A 0.55437
436B -> 438B 0.42866
436B -> 439B 0.55433

Excited State 29: 3.000-A 1.8865 eV 657.21 nm f=0.0000 <S**2>=2.000
404A -> 437A 0.11793
406A -> 437A 0.11593
409A -> 437A 0.12582
413A -> 437A -0.12173
419A -> 437A -0.19381
421A -> 437A 0.14074
422A -> 437A 0.36894
425A -> 437A 0.32491
426A -> 437A -0.13017
427A -> 437A 0.22404
404B -> 437B -0.11793
406B -> 437B -0.11593
409B -> 437B -0.12582
413B -> 437B 0.12173
419B -> 437B 0.19380
421B -> 437B -0.14074
422B -> 437B -0.36894
425B -> 437B -0.32490
426B -> 437B 0.13017

427B -> 437B -0.22404

Excited State 30: 3.000-A 1.9416 eV 638.57 nm f=0.0000 <S**2>=2.000
419A -> 437A 0.16419
422A -> 437A -0.24213
425A -> 437A 0.45073
426A -> 437A -0.14126
427A -> 437A 0.30593
419B -> 437B -0.16419
422B -> 437B 0.24213
425B -> 437B -0.45073
426B -> 437B 0.14126
427B -> 437B -0.30593

Excited State 31: 3.000-A 1.9908 eV 622.77 nm f=0.0000 <S**2>=2.000
433A -> 438A 0.12267
435A -> 438A 0.67481
435A -> 439A 0.12779
433B -> 438B -0.12256
435B -> 438B -0.67417
435B -> 439B -0.12767

Excited State 32: 1.000-A 1.9947 eV 621.58 nm f=0.0000 <S**2>=0.000
433A -> 438A 0.11752
435A -> 438A 0.67705
435A -> 439A 0.12557
433B -> 438B 0.11764
435B -> 438B 0.67769
435B -> 439B 0.12570

Excited State 33: 1.000-A 2.0049 eV 618.39 nm f=0.0121 <S**2>=0.000
425A -> 437A 0.68956
427A -> 437A 0.11878
425B -> 437B 0.68957
427B -> 437B 0.11878

Excited State 34: 3.000-A 2.0539 eV 603.65 nm f=0.0000 <S**2>=2.000
436A -> 440A 0.69596
436B -> 440B -0.69593

Excited State 35: 1.000-A 2.0610 eV 601.57 nm f=0.0001 <S**2>=0.000
436A -> 440A 0.69889
436B -> 440B 0.69891

Excited State 36: 3.000-A 2.1028 eV 589.60 nm f=0.0000 <S**2>=2.000
407A -> 437A -0.22139
408A -> 437A 0.14973
409A -> 437A 0.20705
410A -> 437A -0.16314
415A -> 437A 0.14890
416A -> 437A 0.17705
418A -> 437A -0.11643
419A -> 437A 0.36219
420A -> 437A 0.16297
422A -> 437A 0.23098
407B -> 437B 0.22140
408B -> 437B -0.14972
409B -> 437B -0.20705
410B -> 437B 0.16314
415B -> 437B -0.14890
416B -> 437B -0.17705
418B -> 437B 0.11645
419B -> 437B -0.36219
420B -> 437B -0.16297
422B -> 437B -0.23098

Excited State 37: 3.000-A 2.1403 eV 579.29 nm f=0.0000 <S**2>=2.000
435A -> 438A -0.13545
435A -> 439A 0.69135
435B -> 438B 0.13432
435B -> 439B -0.68543

Excited State 38: 1.000-A 2.1407 eV 579.17 nm f=0.0000 <S**2>=0.000

435A -> 438A -0.13124

435A -> 439A 0.68643

435B -> 438B -0.13239

435B -> 439B 0.69234

Excited State 39: 3.000-A 2.1827 eV 568.04 nm f=0.0000 <S**2>=2.000

407A -> 437A -0.10627

409A -> 437A 0.20208

416A -> 437A -0.11222

420A -> 437A 0.15261

422A -> 437A -0.26880

423A -> 437A 0.52486

407B -> 437B 0.10628

409B -> 437B -0.20208

416B -> 437B 0.11222

420B -> 437B -0.15261

422B -> 437B 0.26879

423B -> 437B -0.52485

Excited State 40: 3.000-A 2.2084 eV 561.43 nm f=0.0000 <S**2>=2.000

404A -> 437A -0.10293

406A -> 437A -0.11461

409A -> 437A -0.20095

413A -> 437A 0.11763

416A -> 437A 0.11944

420A -> 437A -0.19962

422A -> 437A 0.28950

423A -> 437A 0.46197

404B -> 437B 0.10294

406B -> 437B 0.11461

409B -> 437B 0.20095

413B -> 437B -0.11763

416B -> 437B -0.11944

420B -> 437B 0.19962

422B -> 437B -0.28949

423B -> 437B -0.46194

Excited State 41: 1.000-A 2.2190 eV 558.74 nm f=0.0054 <S**2>=0.000
422A -> 437A -0.15344
423A -> 437A 0.68397
422B -> 437B -0.15343
423B -> 437B 0.68400

Excited State 42: 1.000-A 2.2225 eV 557.86 nm f=0.0306 <S**2>=0.000
421A -> 437A 0.12952
422A -> 437A 0.66042
423A -> 437A 0.15554
421B -> 437B 0.12952
422B -> 437B 0.66043
423B -> 437B 0.15555

Excited State 43: 3.000-A 2.2749 eV 545.01 nm f=0.0000 <S**2>=2.000
435A -> 440A 0.69699
435B -> 440B -0.69507

Excited State 44: 1.000-A 2.2763 eV 544.68 nm f=0.0002 <S**2>=0.000
435A -> 440A 0.69668
435B -> 440B 0.69859

Excited State 45: 3.000-A 2.3000 eV 539.06 nm f=0.0000 <S**2>=2.000
397A -> 437A 0.20928
407A -> 437A -0.19143
408A -> 437A 0.12943
409A -> 437A 0.19250
410A -> 437A -0.24837
418A -> 437A 0.13256
419A -> 437A -0.23640
420A -> 437A -0.40216
421A -> 437A 0.12429
397B -> 437B -0.20928
407B -> 437B 0.19144

408B -> 437B -0.12942
409B -> 437B -0.19250
410B -> 437B 0.24837
418B -> 437B -0.13257
419B -> 437B 0.23639
420B -> 437B 0.40217
421B -> 437B -0.12429

Excited State 46: 3.000-A 2.3147 eV 535.63 nm f=0.0000 <S**2>=2.000
402A -> 437A -0.11763
403A -> 437A 0.14386
404A -> 437A 0.18064
405A -> 437A -0.10038
406A -> 437A 0.18220
410A -> 437A 0.21873
416A -> 437A 0.10676
418A -> 437A -0.18341
419A -> 437A 0.19580
420A -> 437A -0.41852
422A -> 437A -0.15278
402B -> 437B 0.11763
403B -> 437B -0.14386
404B -> 437B -0.18064
405B -> 437B 0.10038
406B -> 437B -0.18219
410B -> 437B -0.21873
416B -> 437B -0.10676
418B -> 437B 0.18342
419B -> 437B -0.19579
420B -> 437B 0.41853
422B -> 437B 0.15278

Excited State 47: 1.000-A 2.3264 eV 532.94 nm f=0.0049 <S**2>=0.000
419A -> 437A 0.10604
420A -> 437A 0.66631
421A -> 437A -0.12104

419B -> 437B 0.10605
420B -> 437B 0.66630
421B -> 437B -0.12104

Excited State 48: 3.000-A 2.3924 eV 518.25 nm f=0.0000 <S**2>=2.000
397A -> 437A -0.25319
417A -> 437A 0.14971
420A -> 437A 0.10119
421A -> 437A 0.55662
422A -> 437A -0.21503
397B -> 437B 0.25319
417B -> 437B -0.14970
420B -> 437B -0.10118
421B -> 437B -0.55662
422B -> 437B 0.21503

Excited State 49: 3.000-A 2.3993 eV 516.75 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.12571
433A -> 438A 0.39308
433A -> 439A 0.15898
434A -> 438A -0.50172
434A -> 439A 0.10328
435A -> 438A -0.11671
428B -> 438B -0.12571
433B -> 438B -0.39307
433B -> 439B -0.15898
434B -> 438B 0.50172
434B -> 439B -0.10328
435B -> 438B 0.11671

Excited State 50: 1.000-A 2.4067 eV 515.16 nm f=0.0003 <S**2>=0.000
428A -> 438A -0.11291
433A -> 438A -0.38063
433A -> 439A -0.15660
434A -> 438A 0.52327
434A -> 439A -0.10905

435A -> 438A 0.10740
428B -> 438B -0.11291
433B -> 438B -0.38061
433B -> 439B -0.15660
434B -> 438B 0.52329
434B -> 439B -0.10908
435B -> 438B 0.10739

Excited State 51: 3.000-A 2.4127 eV 513.88 nm f=0.0000 <S**2>=2.000
431A -> 439A 0.15003
433A -> 438A -0.44299
434A -> 438A -0.23802
434A -> 439A 0.40660
431B -> 439B -0.15004
433B -> 438B 0.44304
434B -> 438B 0.23801
434B -> 439B -0.40662

Excited State 52: 1.000-A 2.4141 eV 513.58 nm f=0.0060 <S**2>=0.000
417A -> 437A 0.13042
420A -> 437A 0.10207
421A -> 437A 0.64787
422A -> 437A -0.14583
417B -> 437B 0.13042
420B -> 437B 0.10207
421B -> 437B 0.64787
422B -> 437B -0.14584

Excited State 53: 1.000-A 2.4210 eV 512.12 nm f=0.0002 <S**2>=0.000
431A -> 439A -0.13586
433A -> 438A 0.46858
434A -> 438A 0.24086
434A -> 439A -0.40602
431B -> 439B -0.13585
433B -> 438B 0.46856
434B -> 438B 0.24083

434B -> 439B -0.40599

Excited State 54: 3.000-A 2.4450 eV 507.09 nm f=0.0000 <S**2>=2.000
431A -> 442A 0.12660
434A -> 439A -0.13896
434A -> 442A 0.14896
436A -> 441A 0.29043
436A -> 442A -0.53834
431B -> 442B -0.12660
434B -> 439B 0.13895
434B -> 442B -0.14896
436B -> 441B -0.29043
436B -> 442B 0.53835

Excited State 55: 3.000-A 2.4645 eV 503.08 nm f=0.0000 <S**2>=2.000
396A -> 437A 0.12961
397A -> 437A -0.48024
407A -> 437A -0.10968
409A -> 437A 0.13718
415A -> 437A 0.10579
418A -> 437A -0.24627
420A -> 437A -0.19971
421A -> 437A -0.20259
396B -> 437B -0.12961
397B -> 437B 0.48025
407B -> 437B 0.10969
409B -> 437B -0.13720
415B -> 437B -0.10578
418B -> 437B 0.24633
420B -> 437B 0.19973
421B -> 437B 0.20258

Excited State 56: 1.000-A 2.4654 eV 502.89 nm f=0.0280 <S**2>=0.000
409A -> 437A 0.10465
418A -> 437A -0.34606
419A -> 437A 0.53358

420A -> 437A -0.10564
409B -> 437B 0.10463
418B -> 437B -0.34605
419B -> 437B 0.53357
420B -> 437B -0.10561

Excited State 57: 3.000-A 2.4755 eV 500.84 nm f=0.0000 <S**2>=2.000
431A -> 439A -0.13488
432A -> 438A -0.19907
433A -> 438A -0.25835
433A -> 439A -0.19975
434A -> 438A -0.38760
434A -> 439A -0.40102
431B -> 439B 0.13490
432B -> 438B 0.19909
433B -> 438B 0.25839
433B -> 439B 0.19979
434B -> 438B 0.38766
434B -> 439B 0.40110

Excited State 58: 1.000-A 2.4782 eV 500.30 nm f=0.0001 <S**2>=0.000
431A -> 439A 0.12952
432A -> 438A 0.17523
433A -> 438A 0.25985
433A -> 439A 0.20286
434A -> 438A 0.36583
434A -> 439A 0.45259
431B -> 439B 0.12949
432B -> 438B 0.17520
433B -> 438B 0.25981
433B -> 439B 0.20282
434B -> 438B 0.36577
434B -> 439B 0.45252

Excited State 59: 3.000-A 2.4830 eV 499.32 nm f=0.0000 <S**2>=2.000
407A -> 438A -0.25531

408A -> 438A -0.56111
408A -> 439A -0.20287
411A -> 438A -0.10336
407B -> 438B 0.25527
408B -> 438B 0.56113
408B -> 439B 0.20288
411B -> 438B 0.10337

Excited State 60: 3.000-A 2.4878 eV 498.37 nm f=0.0000 <S**2>=2.000
408A -> 439A 0.12154
410A -> 439A -0.19620
411A -> 438A 0.23557
411A -> 439A -0.57027
408B -> 439B -0.12155
410B -> 439B 0.19619
411B -> 438B -0.23557
411B -> 439B 0.57027

Excited State 61: 3.000-A 2.5001 eV 495.92 nm f=0.0000 <S**2>=2.000
418A -> 437A 0.11138
418A -> 440A 0.57284
419A -> 440A 0.30295
420A -> 440A -0.11645
418B -> 437B -0.11138
418B -> 440B -0.57283
419B -> 440B -0.30298
420B -> 440B 0.11645

Excited State 62: 3.000-A 2.5274 eV 490.56 nm f=0.0000 <S**2>=2.000
411A -> 439A 0.12243
431A -> 439A 0.12526
432A -> 438A 0.34055
432A -> 439A -0.37436
433A -> 438A -0.11570
433A -> 439A 0.29884
434A -> 439A -0.27439

411B -> 439B -0.12243
431B -> 439B -0.12526
432B -> 438B -0.34056
432B -> 439B 0.37436
433B -> 438B 0.11570
433B -> 439B -0.29885
434B -> 439B 0.27439

Excited State 63: 1.000-A 2.5372 eV 488.66 nm f=0.0008 <S**2>=0.000
431A -> 439A 0.11372
432A -> 438A 0.36783
432A -> 439A -0.35334
433A -> 438A -0.11478
433A -> 439A 0.34167
434A -> 439A -0.24526
431B -> 439B 0.11372
432B -> 438B 0.36783
432B -> 439B -0.35333
433B -> 438B -0.11477
433B -> 439B 0.34167
434B -> 439B -0.24526

Excited State 64: 1.000-A 2.5382 eV 488.48 nm f=0.0023 <S**2>=0.000
402A -> 437A 0.13120
403A -> 437A -0.10976
407A -> 437A 0.20974
408A -> 437A -0.15563
409A -> 437A -0.28393
413A -> 437A 0.13494
418A -> 437A 0.34137
419A -> 437A 0.31946
402B -> 437B 0.13120
403B -> 437B -0.10976
407B -> 437B 0.20975
408B -> 437B -0.15562
409B -> 437B -0.28393

413B -> 437B 0.13494
418B -> 437B 0.34136
419B -> 437B 0.31948

Excited State 65: 3.000-A 2.5557 eV 485.13 nm f=0.0000 <S**2>=2.000
402A -> 437A -0.15683
403A -> 437A 0.11833
415A -> 437A 0.27349
416A -> 437A 0.23146
417A -> 437A 0.35585
418A -> 437A 0.25723
419A -> 437A -0.19415
421A -> 437A -0.23160
402B -> 437B 0.15684
403B -> 437B -0.11833
415B -> 437B -0.27349
416B -> 437B -0.23146
417B -> 437B -0.35585
418B -> 437B -0.25724
419B -> 437B 0.19413
421B -> 437B 0.23160

Excited State 66: 3.000-A 2.5727 eV 481.92 nm f=0.0000 <S**2>=2.000
428A -> 441A 0.14348
432A -> 438A 0.21448
433A -> 439A -0.25269
433A -> 441A 0.21379
434A -> 441A -0.11065
435A -> 441A 0.36676
435A -> 442A 0.11564
436A -> 441A 0.24141
436A -> 442A 0.13076
428B -> 441B -0.14348
432B -> 438B -0.21448
433B -> 439B 0.25269
433B -> 441B -0.21380

434B -> 441B 0.11065
435B -> 441B -0.36675
435B -> 442B -0.11564
436B -> 441B -0.24140
436B -> 442B -0.13076

Excited State 67: 1.000-A 2.5770 eV 481.12 nm f=0.0020 <S**2>=0.000
402A -> 437A -0.11027
407A -> 437A -0.14961
408A -> 437A 0.11479
409A -> 437A 0.23785
413A -> 437A -0.10841
415A -> 437A 0.24487
418A -> 437A 0.45509
419A -> 437A 0.19494
420A -> 437A -0.12252
402B -> 437B -0.11026
407B -> 437B -0.14960
408B -> 437B 0.11478
409B -> 437B 0.23790
413B -> 437B -0.10845
415B -> 437B 0.24491
418B -> 437B 0.45535
419B -> 437B 0.19515
420B -> 437B -0.12258

Excited State 68: 3.000-A 2.5794 eV 480.68 nm f=0.0000 <S**2>=2.000
397A -> 437A -0.13844
416A -> 437A -0.18762
418A -> 437A 0.49501
418A -> 440A -0.13154
419A -> 437A 0.34074
420A -> 437A -0.10556
397B -> 437B 0.13842
416B -> 437B 0.18758
418B -> 437B -0.49474

418B -> 440B 0.13154
419B -> 437B -0.34065
420B -> 437B 0.10550

Excited State 69: 1.000-A 2.5853 eV 479.58 nm f=0.0000 <S**2>=0.000
432A -> 438A 0.48182
433A -> 439A -0.47975
434A -> 438A -0.11481
434A -> 439A 0.10106
432B -> 438B 0.48182
433B -> 439B -0.47976
434B -> 438B -0.11481
434B -> 439B 0.10106

Excited State 70: 3.000-A 2.5872 eV 479.23 nm f=0.0000 <S**2>=2.000
431A -> 440A -0.13611
432A -> 438A -0.17002
432A -> 440A -0.13442
433A -> 439A 0.12727
433A -> 440A 0.25385
434A -> 440A 0.51925
436A -> 444A -0.15750
431B -> 440B 0.13611
432B -> 438B 0.17002
432B -> 440B 0.13441
433B -> 439B -0.12727
433B -> 440B -0.25384
434B -> 440B -0.51923
436B -> 444B 0.15750

Excited State 71: 3.000-A 2.5880 eV 479.08 nm f=0.0000 <S**2>=2.000
432A -> 438A 0.39428
433A -> 439A -0.38957
433A -> 441A -0.11633
434A -> 438A -0.10258
434A -> 440A 0.16915

435A -> 441A -0.21260
436A -> 441A -0.15115
432B -> 438B -0.39427
433B -> 439B 0.38956
433B -> 441B 0.11633
434B -> 438B 0.10258
434B -> 440B -0.16915
435B -> 441B 0.21260
436B -> 441B 0.15114

Excited State 72: 3.000-A 2.6035 eV 476.22 nm f=0.0000 <S**2>=2.000
433A -> 440A -0.10154
433A -> 444A -0.12090
434A -> 440A -0.19073
434A -> 444A -0.22524
435A -> 444A 0.10494
436A -> 443A -0.22452
436A -> 444A -0.45415
433B -> 440B 0.10152
433B -> 444B 0.12090
434B -> 440B 0.19069
434B -> 444B 0.22523
435B -> 444B -0.10493
436B -> 443B 0.22453
436B -> 444B 0.45415

Excited State 73: 1.000-A 2.6067 eV 475.64 nm f=0.0012 <S**2>=0.000
431A -> 440A -0.13853
432A -> 440A -0.12103
433A -> 440A 0.27821
434A -> 440A 0.57682
436A -> 441A -0.10917
436A -> 442A 0.12735
431B -> 440B -0.13854
432B -> 440B -0.12104
433B -> 440B 0.27823

434B -> 440B 0.57685
436B -> 441B -0.10917
436B -> 442B 0.12735

Excited State 74: 1.000-A 2.6071 eV 475.56 nm f=0.0146 <S**2>=0.000
414A -> 437A 0.14046
415A -> 437A 0.18216
416A -> 437A 0.19746
417A -> 437A 0.58056
418A -> 437A -0.12646
421A -> 437A -0.12366
414B -> 437B 0.14047
415B -> 437B 0.18217
416B -> 437B 0.19745
417B -> 437B 0.58056
418B -> 437B -0.12644
421B -> 437B -0.12366

Excited State 75: 3.000-A 2.6084 eV 475.32 nm f=0.0000 <S**2>=2.000
431A -> 439A 0.17787
432A -> 438A -0.28214
432A -> 439A -0.48318
433A -> 438A 0.15563
433A -> 439A -0.27858
431B -> 439B -0.17788
432B -> 438B 0.28215
432B -> 439B 0.48319
433B -> 438B -0.15563
433B -> 439B 0.27858

Excited State 76: 1.000-A 2.6146 eV 474.20 nm f=0.0001 <S**2>=0.000
431A -> 439A -0.17695
432A -> 438A 0.27253
432A -> 439A 0.53907
433A -> 438A -0.12953
433A -> 439A 0.23423

431B -> 439B -0.17695
432B -> 438B 0.27253
432B -> 439B 0.53906
433B -> 438B -0.12953
433B -> 439B 0.23423

Excited State 77: 1.000-A 2.6166 eV 473.84 nm f=0.0093 <S**2>=0.000
434A -> 440A -0.14666
436A -> 441A -0.45947
436A -> 442A 0.49405
434B -> 440B -0.14667
436B -> 441B -0.45947
436B -> 442B 0.49405

Excited State 78: 3.000-A 2.6177 eV 473.64 nm f=0.0000 <S**2>=2.000
397A -> 437A 0.12675
409A -> 437A -0.10817
413A -> 437A -0.14894
414A -> 437A 0.48208
415A -> 437A 0.33372
416A -> 437A -0.23672
417A -> 437A -0.10362
418A -> 437A -0.10998
397B -> 437B -0.12675
409B -> 437B 0.10817
413B -> 437B 0.14893
414B -> 437B -0.48207
415B -> 437B -0.33372
416B -> 437B 0.23672
417B -> 437B 0.10363
418B -> 437B 0.10997

Excited State 79: 1.000-A 2.6315 eV 471.16 nm f=0.0011 <S**2>=0.000
406A -> 437A -0.11578
409A -> 437A -0.16022
414A -> 437A 0.30090

415A -> 437A 0.46603
416A -> 437A -0.23442
417A -> 437A -0.16244
418A -> 437A -0.12676
406B -> 437B -0.11578
409B -> 437B -0.16022
414B -> 437B 0.30091
415B -> 437B 0.46604
416B -> 437B -0.23443
417B -> 437B -0.16243
418B -> 437B -0.12676

Excited State 80: 3.000-A 2.6369 eV 470.19 nm f=0.0000 <S**2>=2.000
402A -> 437A 0.14620
403A -> 437A -0.10740
409A -> 437A 0.15564
412A -> 437A 0.15212
414A -> 437A 0.17684
415A -> 437A -0.20907
416A -> 437A -0.22506
417A -> 437A 0.50550
402B -> 437B -0.14620
403B -> 437B 0.10739
409B -> 437B -0.15564
412B -> 437B -0.15211
414B -> 437B -0.17682
415B -> 437B 0.20907
416B -> 437B 0.22504
417B -> 437B -0.50550

Excited State 81: 1.000-A 2.6510 eV 467.69 nm f=0.0135 <S**2>=0.000
397A -> 437A 0.12133
410A -> 437A 0.16686
413A -> 437A -0.18052
414A -> 437A 0.35973
415A -> 437A -0.28115

416A -> 437A -0.33574
417A -> 437A 0.14466
435A -> 443A -0.14833
397B -> 437B 0.12134
410B -> 437B 0.16686
413B -> 437B -0.18052
414B -> 437B 0.35973
415B -> 437B -0.28114
416B -> 437B -0.33576
417B -> 437B 0.14467
435B -> 443B -0.14832

Excited State 82: 3.000-A 2.6557 eV 466.86 nm f=0.0000 <S**2>=2.000
407A -> 437A 0.10740
409A -> 437A 0.14598
410A -> 437A 0.14579
413A -> 437A 0.16305
414A -> 437A -0.36159
415A -> 437A 0.41304
416A -> 437A -0.25618
418A -> 437A -0.10838
407B -> 437B -0.10740
409B -> 437B -0.14599
410B -> 437B -0.14578
413B -> 437B -0.16305
414B -> 437B 0.36160
415B -> 437B -0.41304
416B -> 437B 0.25617
418B -> 437B 0.10838

Excited State 83: 1.000-A 2.6736 eV 463.74 nm f=0.0025 <S**2>=0.000
407A -> 437A -0.16032
409A -> 437A -0.15808
410A -> 437A -0.19698
413A -> 437A -0.19159
414A -> 437A 0.38617

415A -> 437A -0.21100
416A -> 437A 0.33458
417A -> 437A -0.12251
407B -> 437B -0.16033
409B -> 437B -0.15808
410B -> 437B -0.19698
413B -> 437B -0.19160
414B -> 437B 0.38618
415B -> 437B -0.21100
416B -> 437B 0.33459
417B -> 437B -0.12251

Excited State 84: 1.000-A 2.6920 eV 460.56 nm f=0.0009 <S**2>=0.000
435A -> 441A 0.11476
436A -> 441A 0.50840
436A -> 442A 0.45849
435B -> 441B 0.11474
436B -> 441B 0.50846
436B -> 442B 0.45852

Excited State 85: 3.000-A 2.7001 eV 459.18 nm f=0.0000 <S**2>=2.000
433A -> 441A -0.11730
435A -> 441A -0.25252
435A -> 443A -0.13292
436A -> 441A 0.49251
436A -> 442A 0.24096
436A -> 448A -0.12400
433B -> 441B 0.11731
435B -> 441B 0.25252
435B -> 443B 0.13292
436B -> 441B -0.49245
436B -> 442B -0.24090
436B -> 448B 0.12400

Excited State 86: 1.000-A 2.7036 eV 458.60 nm f=0.0238 <S**2>=0.000
402A -> 437A -0.13496

403A -> 437A 0.13619
404A -> 437A 0.16676
406A -> 437A 0.15767
407A -> 437A 0.13583
409A -> 437A -0.15340
410A -> 437A 0.35493
413A -> 437A -0.18239
415A -> 437A 0.17892
416A -> 437A 0.28074
417A -> 437A -0.14114
435A -> 443A -0.12074
402B -> 437B -0.13496
403B -> 437B 0.13620
404B -> 437B 0.16676
406B -> 437B 0.15767
407B -> 437B 0.13583
409B -> 437B -0.15340
410B -> 437B 0.35493
413B -> 437B -0.18238
415B -> 437B 0.17892
416B -> 437B 0.28073
417B -> 437B -0.14114
435B -> 443B -0.12071

Excited State 87: 3.000-A 2.7117 eV 457.23 nm f=0.0000 <S**2>=2.000
431A -> 438A 0.46612
431A -> 439A -0.38689
432A -> 439A -0.25645
434A -> 439A 0.16975
431B -> 438B -0.46611
431B -> 439B 0.38689
432B -> 439B 0.25644
434B -> 439B -0.16975

Excited State 88: 3.000-A 2.7172 eV 456.30 nm f=0.0000 <S**2>=2.000
433A -> 443A 0.10335

435A -> 443A -0.57114
435A -> 444A 0.18191
436A -> 441A -0.14516
436A -> 443A -0.13327
433B -> 443B -0.10335
435B -> 443B 0.57114
435B -> 444B -0.18191
436B -> 441B 0.14516
436B -> 443B 0.13327

Excited State 89: 1.000-A 2.7172 eV 456.29 nm f=0.0000 <S**2>=0.000
431A -> 438A 0.49270
431A -> 439A -0.39067
432A -> 439A -0.22758
434A -> 439A 0.15662
431B -> 438B 0.49271
431B -> 439B -0.39068
432B -> 439B -0.22759
434B -> 439B 0.15663

Excited State 90: 3.000-A 2.7302 eV 454.12 nm f=0.0000 <S**2>=2.000
430A -> 438A 0.12803
432A -> 440A -0.18499
433A -> 440A 0.55011
434A -> 440A -0.34276
430B -> 438B -0.12802
432B -> 440B 0.18496
433B -> 440B -0.54996
434B -> 440B 0.34268

Excited State 91: 3.000-A 2.7307 eV 454.03 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.34021
428A -> 439A 0.10568
429A -> 438A -0.10734
430A -> 438A 0.48936
431A -> 439A 0.13036

432A -> 438A -0.10977
433A -> 438A -0.13211
433A -> 440A -0.14139
428B -> 438B -0.34018
428B -> 439B -0.10568
429B -> 438B 0.10733
430B -> 438B -0.48931
431B -> 439B -0.13035
432B -> 438B 0.10976
433B -> 438B 0.13210
433B -> 440B 0.14135

Excited State 92: 1.000-A 2.7329 eV 453.67 nm f=0.0000 <S**2>=0.000
432A -> 440A -0.11462
433A -> 440A 0.60720
434A -> 440A -0.32699
432B -> 440B -0.11467
433B -> 440B 0.60735
434B -> 440B -0.32708

Excited State 93: 3.000-A 2.7361 eV 453.13 nm f=0.0000 <S**2>=2.000
396A -> 437A 0.17017
402A -> 437A -0.13022
403A -> 437A 0.13682
404A -> 437A 0.11616
405A -> 437A -0.12278
410A -> 437A -0.22874
413A -> 437A 0.50072
414A -> 437A 0.11616
416A -> 437A -0.20018
396B -> 437B -0.17016
402B -> 437B 0.13022
403B -> 437B -0.13682
404B -> 437B -0.11616
405B -> 437B 0.12278
410B -> 437B 0.22874

413B -> 437B -0.50072
414B -> 437B -0.11616
416B -> 437B 0.20018

Excited State 94: 1.000-A 2.7425 eV 452.09 nm f=0.0001 <S**2>=0.000
428A -> 438A 0.33650
428A -> 439A 0.10680
430A -> 438A 0.55054
431A -> 439A 0.15058
433A -> 438A -0.12277
428B -> 438B 0.33653
428B -> 439B 0.10680
430B -> 438B 0.55059
431B -> 439B 0.15059
433B -> 438B -0.12278

Excited State 95: 1.000-A 2.7659 eV 448.27 nm f=0.0022 <S**2>=0.000
404A -> 437A 0.13914
405A -> 437A -0.11636
406A -> 437A 0.11931
412A -> 437A 0.32769
413A -> 437A 0.45969
414A -> 437A 0.23060
417A -> 437A -0.17751
404B -> 437B 0.13914
405B -> 437B -0.11636
406B -> 437B 0.11930
412B -> 437B 0.32769
413B -> 437B 0.45969
414B -> 437B 0.23060
417B -> 437B -0.17751

Excited State 96: 3.000-A 2.7672 eV 448.05 nm f=0.0000 <S**2>=2.000
412A -> 437A 0.21838
431A -> 438A 0.10904
431A -> 439A 0.14266

431A -> 442A -0.10001
432A -> 440A 0.28157
433A -> 440A 0.14673
434A -> 442A -0.12303
436A -> 441A 0.17112
436A -> 443A 0.13232
436A -> 446A 0.10941
436A -> 448A 0.25186
412B -> 437B -0.21838
431B -> 438B -0.10904
431B -> 439B -0.14266
431B -> 442B 0.10001
432B -> 440B -0.28156
433B -> 440B -0.14673
434B -> 442B 0.12303
436B -> 441B -0.17111
436B -> 443B -0.13232
436B -> 446B -0.10941
436B -> 448B -0.25186

Excited State 97: 3.000-A 2.7717 eV 447.33 nm f=0.0000 <S**2>=2.000
407A -> 437A -0.12559
410A -> 437A 0.14018
412A -> 437A 0.50323
414A -> 437A 0.10183
416A -> 437A 0.15437
417A -> 437A -0.15284
432A -> 440A -0.22135
433A -> 440A -0.10822
407B -> 437B 0.12559
410B -> 437B -0.14018
412B -> 437B -0.50323
414B -> 437B -0.10183
416B -> 437B -0.15437
417B -> 437B 0.15283
432B -> 440B 0.22134

433B -> 440B 0.10822

Excited State 98: 3.000-A 2.7768 eV 446.50 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.14003
431A -> 438A -0.40307
431A -> 439A -0.37205
432A -> 440A 0.33500
433A -> 440A 0.14133
428B -> 438B -0.14004
431B -> 438B 0.40307
431B -> 439B 0.37206
432B -> 440B -0.33499
433B -> 440B -0.14133

Excited State 99: 1.000-A 2.7809 eV 445.84 nm f=0.0004 <S**2>=0.000
428A -> 438A -0.15563
431A -> 438A 0.46773
431A -> 439A 0.47118
434A -> 439A -0.10145
428B -> 438B -0.15563
431B -> 438B 0.46772
431B -> 439B 0.47118
434B -> 439B -0.10145

Excited State 100: 3.000-A 2.7842 eV 445.32 nm f=0.0000 <S**2>=2.000
431A -> 438A 0.23918
431A -> 439A 0.20655
432A -> 440A 0.38204
433A -> 440A 0.13415
436A -> 441A -0.11870
436A -> 443A -0.10525
436A -> 448A -0.22837
431B -> 438B -0.23917
431B -> 439B -0.20655
432B -> 440B -0.38203
433B -> 440B -0.13415

436B -> 441B 0.11870
436B -> 443B 0.10525
436B -> 448B 0.22837

Excited State 101: 1.000-A 2.7876 eV 444.78 nm f=0.0039 <S**2>=0.000
402A -> 437A 0.11880
403A -> 437A -0.11512
407A -> 437A -0.13848
410A -> 437A 0.10236
412A -> 437A 0.54413
413A -> 437A -0.28843
414A -> 437A -0.11449
416A -> 437A 0.10053
402B -> 437B 0.11880
403B -> 437B -0.11512
407B -> 437B -0.13849
410B -> 437B 0.10236
412B -> 437B 0.54413
413B -> 437B -0.28843
414B -> 437B -0.11449
416B -> 437B 0.10053

Excited State 102: 1.000-A 2.7969 eV 443.29 nm f=0.0011 <S**2>=0.000
432A -> 440A 0.66833
433A -> 440A 0.16729
432B -> 440B 0.66835
433B -> 440B 0.16729

Excited State 103: 3.000-A 2.8012 eV 442.62 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.20523
429A -> 438A -0.38188
430A -> 438A -0.28788
430A -> 439A 0.43240
432A -> 439A -0.11626
428B -> 438B -0.20523
429B -> 438B 0.38186

430B -> 438B 0.28788
430B -> 439B -0.43240
432B -> 439B 0.11626

Excited State 104: 1.000-A 2.8100 eV 441.23 nm f=0.0076 <S**2>=0.000
433A -> 441A 0.11729
435A -> 441A 0.63780
435A -> 442A 0.15868
433B -> 441B 0.11729
435B -> 441B 0.63780
435B -> 442B 0.15868

Excited State 105: 1.000-A 2.8114 eV 441.00 nm f=0.0003 <S**2>=0.000
428A -> 438A 0.25212
429A -> 438A -0.35039
430A -> 438A -0.24048
430A -> 439A 0.46571
435A -> 441A 0.11908
428B -> 438B 0.25213
429B -> 438B -0.35039
430B -> 438B -0.24048
430B -> 439B 0.46572
435B -> 441B 0.11908

Excited State 106: 3.000-A 2.8145 eV 440.52 nm f=0.0000 <S**2>=2.000
401A -> 437A -0.11596
405A -> 437A 0.20823
406A -> 437A -0.21681
409A -> 437A 0.18265
410A -> 437A 0.33090
411A -> 437A -0.18846
412A -> 437A -0.25282
413A -> 437A 0.28011
414A -> 437A 0.19279
401B -> 437B 0.11596
405B -> 437B -0.20822

406B -> 437B 0.21680
409B -> 437B -0.18264
410B -> 437B -0.33089
411B -> 437B 0.18846
412B -> 437B 0.25281
413B -> 437B -0.28010
414B -> 437B -0.19279

Excited State 107: 3.000-A 2.8241 eV 439.02 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.17964
429A -> 438A 0.36541
429A -> 439A 0.12338
430A -> 439A 0.26167
431A -> 442A -0.13223
434A -> 442A -0.14565
436A -> 442A -0.11107
436A -> 448A -0.11723
436A -> 450A 0.17574
428B -> 438B -0.17963
429B -> 438B -0.36540
429B -> 439B -0.12338
430B -> 439B -0.26166
431B -> 442B 0.13223
434B -> 442B 0.14565
436B -> 442B 0.11107
436B -> 448B 0.11724
436B -> 450B -0.17575

Excited State 108: 1.000-A 2.8291 eV 438.25 nm f=0.0051 <S**2>=0.000
405A -> 437A 0.12672
406A -> 437A -0.11757
410A -> 437A 0.23059
411A -> 437A -0.11583
413A -> 437A 0.12032
436A -> 443A 0.34647
436A -> 444A 0.43932

405B -> 437B 0.12725
406B -> 437B -0.11766
410B -> 437B 0.23103
411B -> 437B -0.11586
413B -> 437B 0.12030
436B -> 443B 0.34652
436B -> 444B 0.43951

Excited State 109: 3.000-A 2.8291 eV 438.25 nm f=0.0000 <S**2>=2.000
402A -> 437A -0.13396
405A -> 437A 0.12425
407A -> 437A -0.26802
409A -> 437A -0.26708
410A -> 437A 0.10268
416A -> 437A -0.19280
429A -> 438A 0.31635
430A -> 439A 0.17545
436A -> 450A -0.10474
402B -> 437B 0.13403
405B -> 437B -0.12368
407B -> 437B 0.26771
409B -> 437B 0.26743
410B -> 437B -0.10166
416B -> 437B 0.19288
429B -> 438B -0.31602
430B -> 439B -0.17536
436B -> 450B 0.10463

Excited State 110: 3.000-A 2.8317 eV 437.84 nm f=0.0000 <S**2>=2.000
407A -> 437A -0.25517
409A -> 437A -0.23553
416A -> 437A -0.16260
429A -> 438A -0.23280
430A -> 439A -0.11910
431A -> 442A -0.13531
434A -> 442A -0.14212

436A -> 442A -0.10077
436A -> 448A -0.10539
436A -> 450A 0.18292
407B -> 437B 0.25526
409B -> 437B 0.23549
416B -> 437B 0.16260
429B -> 438B 0.23273
430B -> 439B 0.11906
431B -> 442B 0.13531
434B -> 442B 0.14212
436B -> 442B 0.10079
436B -> 448B 0.10541
436B -> 450B -0.18292

Excited State 111: 1.000-A 2.8320 eV 437.80 nm f=0.0032 <S**2>=0.000
397A -> 437A -0.11272
405A -> 437A 0.23518
406A -> 437A -0.19482
407A -> 437A -0.17199
410A -> 437A 0.34246
411A -> 437A -0.15773
413A -> 437A 0.14223
436A -> 443A -0.21482
436A -> 444A -0.29764
397B -> 437B -0.11273
405B -> 437B 0.23514
406B -> 437B -0.19483
407B -> 437B -0.17188
410B -> 437B 0.34242
411B -> 437B -0.15773
413B -> 437B 0.14222
436B -> 443B -0.21481
436B -> 444B -0.29761

Excited State 112: 1.000-A 2.8340 eV 437.49 nm f=0.0002 <S**2>=0.000
428A -> 438A 0.18151

429A -> 438A 0.57401
429A -> 439A 0.15408
430A -> 439A 0.28884
428B -> 438B 0.18152
429B -> 438B 0.57405
429B -> 439B 0.15409
430B -> 439B 0.28886

Excited State 113: 3.000-A 2.8397 eV 436.60 nm f=0.0000 <S**2>=2.000
401A -> 437A 0.24327
402A -> 437A 0.23714
405A -> 437A -0.23807
406A -> 437A 0.32072
407A -> 437A -0.24912
410A -> 437A 0.10474
412A -> 437A -0.26049
413A -> 437A 0.14696
401B -> 437B -0.24327
402B -> 437B -0.23714
405B -> 437B 0.23807
406B -> 437B -0.32071
407B -> 437B 0.24911
410B -> 437B -0.10473
412B -> 437B 0.26048
413B -> 437B -0.14696

Excited State 114: 1.000-A 2.8437 eV 435.99 nm f=0.0065 <S**2>=0.000
402A -> 437A 0.17643
403A -> 437A -0.15052
406A -> 437A -0.12634
407A -> 437A 0.33734
408A -> 437A -0.10665
409A -> 437A 0.46573
416A -> 437A 0.20547
402B -> 437B 0.17643
403B -> 437B -0.15052

406B -> 437B -0.12635
407B -> 437B 0.33738
408B -> 437B -0.10664
409B -> 437B 0.46574
416B -> 437B 0.20547

Excited State 115: 3.000-A 2.8635 eV 432.99 nm f=0.0000 <S**2>=2.000
391A -> 438A -0.13698
428A -> 438A 0.41307
428A -> 439A 0.10164
430A -> 438A -0.32969
430A -> 439A -0.37213
391B -> 438B 0.13699
428B -> 438B -0.41306
428B -> 439B -0.10164
430B -> 438B 0.32969
430B -> 439B 0.37212

Excited State 116: 1.000-A 2.8648 eV 432.79 nm f=0.0156 <S**2>=0.000
397A -> 437A 0.10286
401A -> 437A 0.25175
402A -> 437A 0.31109
403A -> 437A -0.15607
405A -> 437A -0.23408
406A -> 437A 0.28672
407A -> 437A -0.24505
410A -> 437A 0.11468
412A -> 437A -0.19163
397B -> 437B 0.10286
401B -> 437B 0.25175
402B -> 437B 0.31109
403B -> 437B -0.15607
405B -> 437B -0.23409
406B -> 437B 0.28673
407B -> 437B -0.24506
410B -> 437B 0.11469

412B -> 437B -0.19163

Excited State 117: 1.000-A 2.8700 eV 431.99 nm f=0.0002 <S**2>=0.000
428A -> 438A 0.46612
428A -> 439A 0.11052
430A -> 438A -0.31384
430A -> 439A -0.38024
428B -> 438B 0.46613
428B -> 439B 0.11053
430B -> 438B -0.31385
430B -> 439B -0.38025

Excited State 118: 3.000-A 2.8937 eV 428.46 nm f=0.0000 <S**2>=2.000
391A -> 438A 0.13677
428A -> 441A 0.21835
430A -> 441A 0.11763
433A -> 441A 0.11972
433A -> 447A 0.14417
434A -> 441A -0.12613
435A -> 441A -0.23698
435A -> 442A -0.12648
435A -> 445A 0.17152
435A -> 447A 0.20076
435A -> 455A -0.13873
391B -> 438B -0.13677
428B -> 441B -0.21835
430B -> 441B -0.11762
433B -> 441B -0.11972
433B -> 447B -0.14417
434B -> 441B 0.12613
435B -> 441B 0.23699
435B -> 442B 0.12648
435B -> 445B -0.17152
435B -> 447B -0.20076
435B -> 455B 0.13873

Excited State 119: 3.000-A 2.9077 eV 426.40 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 390A -> 439A | -0.12477 |
| 391A -> 439A | 0.10000 |
| 392A -> 438A | 0.22526 |
| 392A -> 439A | -0.50963 |
| 404A -> 439A | 0.18648 |
| 390B -> 439B | 0.12477 |
| 391B -> 439B | -0.10001 |
| 392B -> 438B | -0.22526 |
| 392B -> 439B | 0.50963 |
| 404B -> 439B | -0.18648 |

Excited State 120: 3.000-A 2.9107 eV 425.97 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 394A -> 451A | -0.10801 |
| 395A -> 440A | -0.57756 |
| 412A -> 440A | 0.17821 |
| 413A -> 440A | 0.10073 |
| 416A -> 440A | -0.10085 |
| 432A -> 440A | 0.11082 |
| 394B -> 451B | 0.10801 |
| 395B -> 440B | 0.57756 |
| 412B -> 440B | -0.17822 |
| 413B -> 440B | -0.10073 |
| 416B -> 440B | 0.10085 |
| 432B -> 440B | -0.11082 |
| 395A <- 440A | -0.11132 |
| 395B <- 440B | 0.11132 |

Excited State 121: 3.000-A 2.9126 eV 425.68 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 390A -> 438A | -0.16441 |
| 391A -> 438A | 0.46644 |
| 391A -> 439A | 0.16186 |
| 392A -> 439A | 0.11566 |
| 401A -> 438A | 0.15617 |
| 428A -> 438A | 0.19188 |
| 390B -> 438B | 0.16441 |

391B -> 438B -0.46645
391B -> 439B -0.16186
392B -> 439B -0.11566
401B -> 438B -0.15617
428B -> 438B -0.19188

Excited State 122: 1.000-A 2.9277 eV 423.48 nm f=0.0138 <S**2>=0.000
396A -> 437A -0.11906
397A -> 437A 0.38849
435A -> 443A 0.31071
436A -> 443A 0.32062
436A -> 444A -0.27030
396B -> 437B -0.11906
397B -> 437B 0.38849
435B -> 443B 0.31072
436B -> 443B 0.32060
436B -> 444B -0.27029

Excited State 123: 3.000-A 2.9473 eV 420.67 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.23155
433A -> 443A -0.10742
434A -> 442A -0.10564
435A -> 443A 0.10027
436A -> 443A -0.50482
436A -> 444A 0.27754
429B -> 439B 0.23152
433B -> 443B 0.10742
434B -> 442B 0.10564
435B -> 443B -0.10026
436B -> 443B 0.50483
436B -> 444B -0.27754

Excited State 124: 3.000-A 2.9497 eV 420.32 nm f=0.0000 <S**2>=2.000
429A -> 438A -0.10441
429A -> 439A 0.62112
430A -> 439A -0.15581

436A -> 443A -0.20089
429B -> 438B 0.10438
429B -> 439B -0.62094
430B -> 439B 0.15577
436B -> 443B 0.20089

Excited State 125: 1.000-A 2.9516 eV 420.06 nm f=0.0001 <S**2>=0.000
429A -> 438A -0.10137
429A -> 439A 0.66913
430A -> 439A -0.15739
429B -> 438B -0.10140
429B -> 439B 0.66931
430B -> 439B -0.15743

Excited State 126: 3.000-A 2.9754 eV 416.70 nm f=0.0000 <S**2>=2.000
431A -> 442A -0.12384
434A -> 441A 0.11681
434A -> 442A -0.27137
434A -> 444A -0.11890
436A -> 442A -0.17708
436A -> 443A 0.20572
436A -> 444A 0.12318
436A -> 446A -0.19694
436A -> 448A -0.15362
436A -> 450A -0.21014
436A -> 459A -0.10040
431B -> 442B 0.12384
434B -> 441B -0.11681
434B -> 442B 0.27137
434B -> 444B 0.11890
436B -> 442B 0.17708
436B -> 443B -0.20571
436B -> 444B -0.12318
436B -> 446B 0.19694
436B -> 448B 0.15362
436B -> 450B 0.21014

436B -> 459B 0.10040

Excited State 127: 1.000-A 2.9780 eV 416.33 nm f=0.0218 <S**2>=0.000
396A -> 437A 0.10732
397A -> 437A -0.27361
435A -> 443A -0.26621
436A -> 443A 0.44887
436A -> 444A -0.32902
396B -> 437B 0.10732
397B -> 437B -0.27362
435B -> 443B -0.26621
436B -> 443B 0.44888
436B -> 444B -0.32902

Excited State 128: 3.000-A 2.9864 eV 415.16 nm f=0.0000 <S**2>=2.000
428A -> 439A -0.36293
433A -> 442A 0.10888
435A -> 441A -0.28716
435A -> 442A 0.40584
428B -> 439B 0.36286
433B -> 442B -0.10887
435B -> 441B 0.28715
435B -> 442B -0.40576

Excited State 129: 3.000-A 2.9899 eV 414.68 nm f=0.0000 <S**2>=2.000
408A -> 437A 0.12913
410A -> 437A 0.21388
411A -> 437A 0.64343
408B -> 437B -0.12906
410B -> 437B -0.21374
411B -> 437B -0.64305

Excited State 130: 1.000-A 2.9903 eV 414.62 nm f=0.0000 <S**2>=0.000
408A -> 437A 0.12846
410A -> 437A 0.22698
411A -> 437A 0.64063

408B -> 437B 0.12855
410B -> 437B 0.22711
411B -> 437B 0.64102

Excited State 131: 1.000-A 2.9909 eV 414.54 nm f=0.0005 <S**2>=0.000
428A -> 438A -0.14078
428A -> 439A 0.67752
428B -> 438B -0.14075
428B -> 439B 0.67735

Excited State 132: 3.000-A 2.9932 eV 414.21 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.12447
428A -> 439A -0.55676
435A -> 441A 0.18530
435A -> 442A -0.30071
428B -> 438B -0.12452
428B -> 439B 0.55701
435B -> 441B -0.18528
435B -> 442B 0.30063

Excited State 133: 1.000-A 3.0083 eV 412.14 nm f=0.0024 <S**2>=0.000
435A -> 441A -0.17395
435A -> 442A 0.66536
435B -> 441B -0.17401
435B -> 442B 0.66543

Excited State 134: 3.000-A 3.0199 eV 410.56 nm f=0.0000 <S**2>=2.000
430A -> 440A -0.12432
431A -> 440A -0.38850
431A -> 444A 0.11823
433A -> 444A -0.11502
434A -> 443A -0.12248
434A -> 444A -0.23206
434A -> 448A -0.13659
436A -> 444A 0.25764
436A -> 450A 0.13377

430B -> 440B 0.12433
431B -> 440B 0.38852
431B -> 444B -0.11823
433B -> 444B 0.11502
434B -> 443B 0.12248
434B -> 444B 0.23206
434B -> 448B 0.13659
436B -> 444B -0.25764
436B -> 450B -0.13377

Excited State 135: 3.000-A 3.0277 eV 409.50 nm f=0.0000 <S**2>=2.000
407A -> 437A -0.30133
408A -> 437A -0.60157
409A -> 437A 0.11504
411A -> 437A 0.14746
407B -> 437B 0.30151
408B -> 437B 0.60206
409B -> 437B -0.11512
411B -> 437B -0.14758

Excited State 136: 1.000-A 3.0281 eV 409.45 nm f=0.0000 <S**2>=0.000
407A -> 437A 0.29728
408A -> 437A 0.60933
409A -> 437A -0.10958
411A -> 437A -0.14430
407B -> 437B 0.29701
408B -> 437B 0.60889
409B -> 437B -0.10950
411B -> 437B -0.14419

Excited State 137: 1.000-A 3.0293 eV 409.29 nm f=0.0001 <S**2>=0.000
418A -> 440A 0.10621
430A -> 440A 0.18089
431A -> 440A 0.65297
434A -> 440A 0.10568
418B -> 440B 0.10621

430B -> 440B 0.18091
431B -> 440B 0.65307
434B -> 440B 0.10570

Excited State 138: 3.000-A 3.0315 eV 408.99 nm f=0.0000 <S**2>=2.000
430A -> 440A 0.15349
431A -> 440A 0.52140
434A -> 444A -0.17985
436A -> 444A 0.19270
436A -> 450A 0.10340
430B -> 440B -0.15345
431B -> 440B -0.52126
434B -> 444B 0.17985
436B -> 444B -0.19269
436B -> 450B -0.10339

Excited State 139: 1.000-A 3.0480 eV 406.78 nm f=0.0000 <S**2>=0.000
407A -> 438A 0.25592
408A -> 438A 0.56270
408A -> 439A 0.21176
411A -> 438A 0.13017
407B -> 438B 0.25588
408B -> 438B 0.56272
408B -> 439B 0.21176
411B -> 438B 0.13017

Excited State 140: 3.000-A 3.0525 eV 406.18 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.11152
428A -> 441A 0.15888
433A -> 441A 0.17189
433A -> 445A -0.10016
433A -> 447A -0.11254
434A -> 441A -0.14684
435A -> 441A -0.15174
435A -> 442A -0.38439
435A -> 445A -0.13084

435A -> 447A -0.18058
398B -> 437B -0.11152
428B -> 441B -0.15889
433B -> 441B -0.17189
433B -> 445B 0.10016
433B -> 447B 0.11254
434B -> 441B 0.14684
435B -> 441B 0.15173
435B -> 442B 0.38442
435B -> 445B 0.13084
435B -> 447B 0.18058

Excited State 141: 1.000-A 3.0539 eV 405.99 nm f=0.0000 <S**2>=0.000
408A -> 439A -0.10237
410A -> 439A 0.20297
411A -> 438A -0.23705
411A -> 439A 0.59047
408B -> 439B -0.10237
410B -> 439B 0.20297
411B -> 438B -0.23705
411B -> 439B 0.59048

Excited State 142: 1.000-A 3.0593 eV 405.27 nm f=0.0000 <S**2>=0.000
418A -> 440A 0.50072
419A -> 440A 0.27242
420A -> 440A -0.10700
430A -> 440A 0.30182
431A -> 440A -0.18761
418B -> 440B 0.50071
419B -> 440B 0.27244
420B -> 440B -0.10700
430B -> 440B 0.30180
431B -> 440B -0.18759

Excited State 143: 3.000-A 3.0613 eV 405.01 nm f=0.0000 <S**2>=2.000
405A -> 437A -0.11441

406A -> 437A -0.10667
428A -> 440A 0.16425
430A -> 440A -0.61188
431A -> 440A 0.17837
432A -> 440A -0.12473
405B -> 437B 0.11440
406B -> 437B 0.10667
428B -> 440B -0.16425
430B -> 440B 0.61190
431B -> 440B -0.17837
432B -> 440B 0.12473

Excited State 144: 3.000-A 3.0621 eV 404.90 nm f=0.0000 <S**2>=2.000
396A -> 437A -0.12304
398A -> 437A 0.20765
405A -> 437A 0.40914
406A -> 437A 0.39737
410A -> 437A -0.10963
430A -> 440A -0.16318
396B -> 437B 0.12304
398B -> 437B -0.20764
405B -> 437B -0.40911
406B -> 437B -0.39734
410B -> 437B 0.10962
430B -> 440B 0.16318

Excited State 145: 1.000-A 3.0665 eV 404.32 nm f=0.0003 <S**2>=0.000
398A -> 437A 0.12973
404A -> 437A -0.18585
405A -> 437A 0.41881
406A -> 437A 0.47637
407A -> 437A 0.11434
398B -> 437B 0.12970
404B -> 437B -0.18583
405B -> 437B 0.41885
406B -> 437B 0.47639

407B -> 437B 0.11435

Excited State 146: 3.000-A 3.0670 eV 404.25 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.13548
396A -> 437A -0.16096
397A -> 437A -0.12458
398A -> 437A -0.38003
402A -> 437A 0.34494
403A -> 437A 0.18491
404A -> 437A 0.25319
405A -> 437A 0.10446
393B -> 437B 0.13548
396B -> 437B 0.16095
397B -> 437B 0.12457
398B -> 437B 0.38004
402B -> 437B -0.34492
403B -> 437B -0.18490
404B -> 437B -0.25320
405B -> 437B -0.10440

Excited State 147: 3.000-A 3.0716 eV 403.65 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.10468
398A -> 437A 0.31166
401A -> 437A 0.13579
402A -> 437A 0.22537
403A -> 437A 0.45798
406A -> 437A -0.23899
393B -> 437B -0.10468
398B -> 437B -0.31164
401B -> 437B -0.13576
402B -> 437B -0.22522
403B -> 437B -0.45780
406B -> 437B 0.23899

Excited State 148: 1.000-A 3.0725 eV 403.52 nm f=0.0002 <S**2>=0.000
402A -> 437A 0.41664

403A -> 437A 0.47986
404A -> 437A 0.12080
405A -> 437A 0.25011
402B -> 437B 0.41674
403B -> 437B 0.48004
404B -> 437B 0.12084
405B -> 437B 0.25012

Excited State 149: 1.000-A 3.0742 eV 403.31 nm f=0.0001 <S**2>=0.000
418A -> 440A -0.29647
419A -> 440A -0.15221
428A -> 440A -0.13575
430A -> 440A 0.57777
418B -> 440B -0.29646
419B -> 440B -0.15222
428B -> 440B -0.13575
430B -> 440B 0.57778

Excited State 150: 1.000-A 3.0818 eV 402.31 nm f=0.0001 <S**2>=0.000
401A -> 437A 0.12848
403A -> 437A -0.32433
404A -> 437A 0.55108
405A -> 437A 0.23027
401B -> 437B 0.12836
403B -> 437B -0.32410
404B -> 437B 0.55067
405B -> 437B 0.23016

Excited State 151: 3.000-A 3.0825 eV 402.22 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.18316
401A -> 437A -0.16525
403A -> 437A 0.30892
404A -> 437A -0.54399
405A -> 437A -0.14348
398B -> 437B 0.18310
401B -> 437B 0.16535

403B -> 437B -0.30917
404B -> 437B 0.54440
405B -> 437B 0.14365

Excited State 152: 3.000-A 3.0885 eV 401.44 nm f=0.0000 <S**2>=2.000
396A -> 437A 0.10015
398A -> 437A -0.27916
401A -> 437A 0.46343
402A -> 437A -0.12591
405A -> 437A 0.28377
433A -> 443A -0.13278
435A -> 449A 0.12495
396B -> 437B -0.10015
398B -> 437B 0.27914
401B -> 437B -0.46341
402B -> 437B 0.12589
405B -> 437B -0.28376
433B -> 443B 0.13277
435B -> 449B -0.12495

Excited State 153: 1.000-A 3.0947 eV 400.63 nm f=0.0010 <S**2>=0.000
401A -> 437A 0.60205
402A -> 437A -0.29002
403A -> 437A 0.11513
401B -> 437B 0.60205
402B -> 437B -0.29002
403B -> 437B 0.11513

Excited State 154: 3.000-A 3.1013 eV 399.78 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.10846
396A -> 437A 0.11385
401A -> 437A -0.33094
402A -> 437A 0.22915
433A -> 443A -0.26826
434A -> 443A 0.14372
435A -> 449A 0.24739

393B -> 437B -0.10847
396B -> 437B -0.11385
401B -> 437B 0.33098
402B -> 437B -0.22916
433B -> 443B 0.26825
434B -> 443B -0.14371
435B -> 449B -0.24739

Excited State 155: 1.000-A 3.1023 eV 399.65 nm f=0.0026 <S**2>=0.000
398A -> 437A 0.64888
399A -> 437A -0.10696
400A -> 437A -0.13804
404A -> 437A 0.12123
398B -> 437B 0.64891
399B -> 437B -0.10695
400B -> 437B -0.13805
404B -> 437B 0.12122

Excited State 156: 3.000-A 3.1314 eV 395.94 nm f=0.0000 <S**2>=2.000
426A -> 438A 0.58315
426A -> 439A 0.11771
427A -> 438A 0.34541
426B -> 438B -0.58310
426B -> 439B -0.11770
427B -> 438B -0.34537

Excited State 157: 1.000-A 3.1341 eV 395.60 nm f=0.1097 <S**2>=0.000
397A -> 437A -0.36046
405A -> 437A -0.11284
407A -> 437A 0.10056
433A -> 443A 0.14881
435A -> 443A 0.42847
397B -> 437B -0.36046
405B -> 437B -0.11285
407B -> 437B 0.10056
433B -> 443B 0.14881

435B -> 443B 0.42846

Excited State 158: 1.000-A 3.1434 eV 394.42 nm f=0.0006 <S**2>=0.000
426A -> 438A 0.58001
426A -> 439A 0.11165
427A -> 438A 0.37028
426B -> 438B 0.58006
426B -> 439B 0.11166
427B -> 438B 0.37031

Excited State 159: 3.000-A 3.1493 eV 393.69 nm f=0.0000 <S**2>=2.000
428A -> 440A 0.12343
429A -> 440A 0.63605
432A -> 442A -0.16353
428B -> 440B -0.12341
429B -> 440B -0.63597
432B -> 442B 0.16353

Excited State 160: 1.000-A 3.1556 eV 392.91 nm f=0.0003 <S**2>=0.000
428A -> 440A 0.13146
429A -> 440A 0.68297
428B -> 440B 0.13147
429B -> 440B 0.68303

Excited State 161: 3.000-A 3.1587 eV 392.52 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.14969
396A -> 437A 0.33573
402A -> 437A 0.12766
429A -> 440A 0.14111
431A -> 442A -0.15829
432A -> 441A -0.13857
432A -> 442A 0.28503
435A -> 444A -0.12934
435A -> 449A -0.14458
393B -> 437B -0.14969
396B -> 437B -0.33573

402B -> 437B -0.12766
429B -> 440B -0.14115
431B -> 442B 0.15829
432B -> 441B 0.13857
432B -> 442B -0.28503
435B -> 444B 0.12933
435B -> 449B 0.14458

Excited State 162: 3.000-A 3.1624 eV 392.06 nm f=0.0000 <S**2>=2.000
396A -> 437A 0.24774
429A -> 440A -0.19788
431A -> 442A 0.16810
432A -> 441A 0.14269
432A -> 442A -0.29616
434A -> 442A -0.10726
435A -> 443A -0.13141
435A -> 444A -0.26527
435A -> 449A -0.17543
396B -> 437B -0.24774
429B -> 440B 0.19790
431B -> 442B -0.16810
432B -> 441B -0.14269
432B -> 442B 0.29616
434B -> 442B 0.10726
435B -> 443B 0.13141
435B -> 444B 0.26523
435B -> 449B 0.17542

Excited State 163: 3.000-A 3.1666 eV 391.54 nm f=0.0000 <S**2>=2.000
390A -> 437A -0.10558
393A -> 437A -0.24986
396A -> 437A -0.11122
398A -> 437A 0.10713
432A -> 441A -0.11644
432A -> 442A 0.11853
433A -> 443A -0.30385

433A -> 449A 0.12914
434A -> 443A 0.11432
434A -> 444A -0.10428
435A -> 443A -0.18947
435A -> 444A -0.22605
435A -> 449A -0.10232
390B -> 437B 0.10558
393B -> 437B 0.24986
396B -> 437B 0.11121
398B -> 437B -0.10713
432B -> 441B 0.11644
432B -> 442B -0.11853
433B -> 443B 0.30386
433B -> 449B -0.12914
434B -> 443B -0.11432
434B -> 444B 0.10428
435B -> 443B 0.18948
435B -> 444B 0.22601
435B -> 449B 0.10232

Excited State 164: 1.000-A 3.1824 eV 389.59 nm f=0.0042 <S**2>=0.000
435A -> 443A 0.12909
435A -> 444A 0.63445
436A -> 446A -0.15891
436A -> 448A -0.11916
435B -> 443B 0.12909
435B -> 444B 0.63435
436B -> 446B -0.15891
436B -> 448B -0.11916

Excited State 165: 3.000-A 3.1901 eV 388.65 nm f=0.0000 <S**2>=2.000
390A -> 437A 0.10299
393A -> 437A 0.16600
396A -> 437A -0.22966
435A -> 444A -0.47991
435A -> 449A 0.16759

390B -> 437B -0.10299
393B -> 437B -0.16600
396B -> 437B 0.22966
435B -> 444B 0.48006
435B -> 449B -0.16758

Excited State 166: 1.000-A 3.1989 eV 387.59 nm f=0.0111 <S**2>=0.000
432A -> 441A 0.10142
432A -> 442A -0.11562
434A -> 441A 0.15002
434A -> 442A -0.13665
435A -> 444A 0.24031
436A -> 445A 0.22767
436A -> 446A 0.44893
436A -> 448A 0.24658
432B -> 441B 0.10142
432B -> 442B -0.11562
434B -> 441B 0.15002
434B -> 442B -0.13665
435B -> 444B 0.24036
436B -> 445B 0.22767
436B -> 446B 0.44894
436B -> 448B 0.24658

Excited State 167: 3.000-A 3.2051 eV 386.84 nm f=0.0000 <S**2>=2.000
426A -> 438A -0.26142
427A -> 438A 0.48213
427A -> 439A -0.42349
426B -> 438B 0.26136
427B -> 438B -0.48204
427B -> 439B 0.42340

Excited State 168: 1.000-A 3.2074 eV 386.56 nm f=0.0000 <S**2>=0.000
426A -> 438A -0.28969
427A -> 438A 0.47312
427A -> 439A -0.42914

426B -> 438B -0.28974
427B -> 438B 0.47321
427B -> 439B -0.42923

Excited State 169: 3.000-A 3.2138 eV 385.79 nm f=0.0000 <S**2>=2.000
399A -> 437A -0.23482
400A -> 437A 0.62113
399B -> 437B 0.23442
400B -> 437B -0.62008

Excited State 170: 1.000-A 3.2140 eV 385.76 nm f=0.0004 <S**2>=0.000
399A -> 437A -0.24793
400A -> 437A 0.63845
399B -> 437B -0.24831
400B -> 437B 0.63946

Excited State 171: 3.000-A 3.2183 eV 385.24 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.11954
429A -> 441A 0.21630
432A -> 441A -0.33466
432A -> 442A -0.13938
433A -> 441A -0.20165
434A -> 441A -0.36013
434A -> 442A -0.15343
400B -> 437B -0.11954
429B -> 441B -0.21630
432B -> 441B 0.33467
432B -> 442B 0.13937
433B -> 441B 0.20166
434B -> 441B 0.36015
434B -> 442B 0.15343

Excited State 172: 1.000-A 3.2299 eV 383.86 nm f=0.0596 <S**2>=0.000
432A -> 441A 0.26610
434A -> 441A 0.52443
434A -> 442A -0.14231

436A -> 445A -0.17737
436A -> 448A -0.12917
432B -> 441B 0.26608
434B -> 441B 0.52441
434B -> 442B -0.14231
436B -> 445B -0.17736
436B -> 448B -0.12917

Excited State 173: 3.000-A 3.2345 eV 383.31 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.16356
396A -> 437A 0.15243
398A -> 437A 0.14486
399A -> 437A 0.55040
400A -> 437A 0.15084
435A -> 449A 0.11349
393B -> 437B 0.16356
396B -> 437B -0.15241
398B -> 437B -0.14486
399B -> 437B -0.55035
400B -> 437B -0.15082
435B -> 449B -0.11349

Excited State 174: 1.000-A 3.2382 eV 382.88 nm f=0.0018 <S**2>=0.000
398A -> 437A 0.14065
399A -> 437A 0.63578
400A -> 437A 0.22184
398B -> 437B 0.14065
399B -> 437B 0.63580
400B -> 437B 0.22184

Excited State 175: 3.000-A 3.2428 eV 382.34 nm f=0.0000 <S**2>=2.000
390A -> 437A -0.13939
393A -> 437A -0.30227
394A -> 437A 0.11400
396A -> 437A 0.20862
399A -> 437A -0.33011

400A -> 437A -0.19736
435A -> 444A -0.10580
435A -> 449A 0.16892
436A -> 445A -0.12276
390B -> 437B 0.13939
393B -> 437B 0.30227
394B -> 437B -0.11401
396B -> 437B -0.20858
399B -> 437B 0.33014
400B -> 437B 0.19737
435B -> 444B 0.10580
435B -> 449B -0.16892
436B -> 445B 0.12276

Excited State 176: 1.000-A 3.2516 eV 381.30 nm f=0.0070 <S**2>=0.000
396A -> 437A 0.60798
397A -> 437A 0.16332
434A -> 442A -0.16504
396B -> 437B 0.60798
397B -> 437B 0.16332
434B -> 442B -0.16504

Excited State 177: 3.000-A 3.2528 eV 381.16 nm f=0.0000 <S**2>=2.000
431A -> 448A 0.10830
436A -> 443A -0.10963
436A -> 445A 0.39804
436A -> 446A 0.15066
436A -> 450A -0.11449
436A -> 455A -0.18909
436A -> 458A 0.10633
436A -> 467A 0.11587
436A -> 472A 0.10979
431B -> 448B -0.10829
436B -> 443B 0.10963
436B -> 445B -0.39802
436B -> 446B -0.15065

436B -> 450B 0.11448
436B -> 455B 0.18909
436B -> 458B -0.10633
436B -> 467B -0.11587
436B -> 472B -0.10979

Excited State 178: 3.000-A 3.2599 eV 380.34 nm f=0.0000 <S**2>=2.000
426A -> 438A -0.23343
427A -> 438A 0.35767
427A -> 439A 0.54339
426B -> 438B 0.23334
427B -> 438B -0.35756
427B -> 439B -0.54321

Excited State 179: 1.000-A 3.2614 eV 380.15 nm f=0.0001 <S**2>=0.000
426A -> 438A -0.25378
427A -> 438A 0.34698
427A -> 439A 0.55550
426B -> 438B -0.25386
427B -> 438B 0.34710
427B -> 439B 0.55568

Excited State 180: 3.000-A 3.2629 eV 379.98 nm f=0.0000 <S**2>=2.000
428A -> 440A 0.66027
429A -> 440A -0.13396
430A -> 440A 0.19409
428B -> 440B -0.65921
429B -> 440B 0.13376
430B -> 440B -0.19380

Excited State 181: 1.000-A 3.2639 eV 379.87 nm f=0.0000 <S**2>=0.000
428A -> 440A 0.66736
429A -> 440A -0.12537
430A -> 440A 0.18049
428B -> 440B 0.66841
429B -> 440B -0.12558

430B -> 440B 0.18079

Excited State 182: 1.000-A 3.2729 eV 378.82 nm f=0.0097 <S**2>=0.000
396A -> 437A 0.19976
432A -> 441A 0.12304
432A -> 442A 0.23805
434A -> 441A 0.25735
434A -> 442A 0.42720
436A -> 445A 0.20852
436A -> 446A -0.12740
436A -> 448A 0.12987
396B -> 437B 0.19976
432B -> 441B 0.12304
432B -> 442B 0.23805
434B -> 441B 0.25734
434B -> 442B 0.42721
436B -> 445B 0.20859
436B -> 446B -0.12754
436B -> 448B 0.12990

Excited State 183: 3.000-A 3.2734 eV 378.76 nm f=0.0000 <S**2>=2.000
436A -> 445A -0.26892
436A -> 446A 0.57512
436A -> 448A -0.10334
436B -> 445B 0.26887
436B -> 446B -0.57509
436B -> 448B 0.10331

Excited State 184: 3.000-A 3.2846 eV 377.47 nm f=0.0000 <S**2>=2.000
426A -> 439A 0.63543
426B -> 439B -0.63534

Excited State 185: 1.000-A 3.2885 eV 377.02 nm f=0.0239 <S**2>=0.000
426A -> 439A -0.18564
432A -> 442A -0.14421
434A -> 442A -0.21853

436A -> 445A 0.49772
436A -> 446A -0.33971
426B -> 439B -0.18567
432B -> 442B -0.14421
434B -> 442B -0.21853
436B -> 445B 0.49771
436B -> 446B -0.33970

Excited State 186: 1.000-A 3.2909 eV 376.75 nm f=0.0014 <S**2>=0.000
426A -> 439A 0.66507
427A -> 438A -0.11074
436A -> 445A 0.15624
426B -> 439B 0.66514
427B -> 438B -0.11075
436B -> 445B 0.15624

Excited State 187: 1.000-A 3.3122 eV 374.32 nm f=0.0448 <S**2>=0.000
433A -> 441A 0.64751
433A -> 442A 0.11005
435A -> 441A -0.12677
433B -> 441B 0.64752
433B -> 442B 0.11005
435B -> 441B -0.12677

Excited State 188: 3.000-A 3.3184 eV 373.63 nm f=0.0000 <S**2>=2.000
394A -> 440A -0.14253
415A -> 440A -0.10888
429A -> 443A 0.10318
432A -> 443A -0.23867
432A -> 444A -0.18566
432A -> 448A -0.12582
434A -> 443A -0.11047
436A -> 445A 0.31536
436A -> 447A -0.12791
436A -> 448A -0.10683
436A -> 455A 0.10435

394B -> 440B 0.14253
415B -> 440B 0.10888
429B -> 443B -0.10318
432B -> 443B 0.23867
432B -> 444B 0.18566
432B -> 448B 0.12582
434B -> 443B 0.11047
436B -> 445B -0.31535
436B -> 447B 0.12791
436B -> 448B 0.10683
436B -> 455B -0.10435

Excited State 189: 3.000-A 3.3242 eV 372.97 nm f=0.0000 <S**2>=2.000
381A -> 439A 0.10779
385A -> 438A -0.10357
386A -> 438A -0.22761
388A -> 439A 0.24985
399A -> 438A -0.21033
400A -> 439A 0.19811
403A -> 438A 0.16595
404A -> 439A -0.10871
405A -> 439A 0.10536
406A -> 439A 0.13136
381B -> 439B -0.10779
385B -> 438B 0.10357
386B -> 438B 0.22761
388B -> 439B -0.24985
399B -> 438B 0.21033
400B -> 439B -0.19811
403B -> 438B -0.16595
404B -> 439B 0.10871
405B -> 439B -0.10536
406B -> 439B -0.13136

Excited State 190: 3.000-A 3.3254 eV 372.84 nm f=0.0000 <S**2>=2.000
388A -> 439A 0.11186

393A -> 440A 0.12206
394A -> 440A 0.29240
395A -> 451A 0.10943
400A -> 439A 0.11212
409A -> 440A 0.10142
413A -> 440A 0.10918
415A -> 440A 0.22776
417A -> 440A 0.11465
426A -> 439A -0.13714
427A -> 440A 0.12243
436A -> 445A 0.10548
388B -> 439B -0.11186
393B -> 440B -0.12206
394B -> 440B -0.29240
395B -> 451B -0.10943
400B -> 439B -0.11212
409B -> 440B -0.10142
413B -> 440B -0.10918
415B -> 440B -0.22776
417B -> 440B -0.11465
426B -> 439B 0.13715
427B -> 440B -0.12243
436B -> 445B -0.10547

Excited State 191: 1.000-A 3.3257 eV 372.81 nm f=0.0139 <S**2>=0.000
432A -> 442A -0.11479
436A -> 445A -0.23174
436A -> 446A -0.27221
436A -> 447A 0.15399
436A -> 448A 0.48756
436A -> 450A -0.13539
432B -> 442B -0.11479
436B -> 445B -0.23175
436B -> 446B -0.27221
436B -> 447B 0.15399
436B -> 448B 0.48757

436B -> 450B -0.13538

Excited State 192: 3.000-A 3.3259 eV 372.79 nm f=0.0000 <S**2>=2.000
386A -> 438A 0.13978
386A -> 439A 0.11628
388A -> 438A -0.14245
388A -> 439A 0.12238
394A -> 440A -0.18007
399A -> 438A 0.15132
400A -> 439A 0.13224
401A -> 438A -0.10006
403A -> 438A -0.15123
415A -> 440A -0.14137
426A -> 439A -0.20026
386B -> 438B -0.13978
386B -> 439B -0.11628
388B -> 438B 0.14245
388B -> 439B -0.12238
394B -> 440B 0.18007
399B -> 438B -0.15132
400B -> 439B -0.13224
401B -> 438B 0.10006
403B -> 438B 0.15123
415B -> 440B 0.14137
426B -> 439B 0.20027

Excited State 193: 3.000-A 3.3354 eV 371.73 nm f=0.0000 <S**2>=2.000
429A -> 443A 0.13306
432A -> 443A -0.20185
433A -> 441A -0.14906
434A -> 443A -0.13815
435A -> 449A 0.10244
436A -> 445A -0.30003
436A -> 447A 0.13178
436A -> 455A -0.18534
436A -> 467A 0.11492

429B -> 443B -0.13306
432B -> 443B 0.20185
433B -> 441B 0.14905
434B -> 443B 0.13815
435B -> 449B -0.10244
436B -> 445B 0.30003
436B -> 447B -0.13178
436B -> 455B 0.18534
436B -> 467B -0.11492

Excited State 194: 3.000-A 3.3506 eV 370.04 nm f=0.0000 <S**2>=2.000
428A -> 443A -0.11211
429A -> 443A -0.23868
431A -> 442A -0.10568
432A -> 441A 0.10931
432A -> 444A -0.30843
433A -> 441A -0.17750
434A -> 441A -0.15478
434A -> 444A -0.11317
435A -> 452A -0.18745
428B -> 443B 0.11211
429B -> 443B 0.23868
431B -> 442B 0.10568
432B -> 441B -0.10931
432B -> 444B 0.30843
433B -> 441B 0.17750
434B -> 441B 0.15478
434B -> 444B 0.11317
435B -> 452B 0.18745

Excited State 195: 3.000-A 3.3585 eV 369.17 nm f=0.0000 <S**2>=2.000
429A -> 441A 0.19716
429A -> 442A 0.13326
430A -> 441A -0.19394
432A -> 441A -0.15729
432A -> 442A -0.12528

| | |
|---|---|
| 432A -> 444A | -0.28445 |
| 433A -> 441A | 0.26617 |
| 434A -> 441A | 0.20601 |
| 429B -> 441B | -0.19716 |
| 429B -> 442B | -0.13326 |
| 430B -> 441B | 0.19394 |
| 432B -> 441B | 0.15729 |
| 432B -> 442B | 0.12528 |
| 432B -> 444B | 0.28445 |
| 433B -> 441B | -0.26617 |
| 434B -> 441B | -0.20601 |

Excited State 196: 3.000-A 3.3718 eV 367.71 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 429A -> 441A | 0.15844 |
| 430A -> 442A | -0.35704 |
| 431A -> 441A | 0.10744 |
| 431A -> 442A | -0.17581 |
| 433A -> 442A | 0.27669 |
| 434A -> 442A | 0.21913 |
| 429B -> 441B | -0.15845 |
| 430B -> 442B | 0.35704 |
| 431B -> 441B | -0.10744 |
| 431B -> 442B | 0.17581 |
| 433B -> 442B | -0.27669 |
| 434B -> 442B | -0.21913 |

Excited State 197: 1.000-A 3.3848 eV 366.30 nm f=0.0129 <S**2>=0.000

| | |
|---|---|
| 432A -> 441A | 0.44318 |
| 432A -> 442A | -0.17443 |
| 433A -> 441A | -0.10288 |
| 433A -> 442A | 0.24101 |
| 434A -> 441A | -0.24575 |
| 435A -> 445A | -0.18883 |
| 436A -> 450A | 0.18765 |
| 432B -> 441B | 0.44318 |
| 432B -> 442B | -0.17444 |

433B -> 441B -0.10286
433B -> 442B 0.24102
434B -> 441B -0.24576
435B -> 445B -0.18882
436B -> 450B 0.18764

Excited State 198: 3.000-A 3.3872 eV 366.03 nm f=0.0000 <S**2>=2.000
428A -> 441A 0.19905
428A -> 442A 0.10999
429A -> 441A 0.20192
430A -> 441A 0.15795
432A -> 441A -0.16933
433A -> 441A -0.24192
434A -> 441A 0.34499
428B -> 441B -0.19905
428B -> 442B -0.10999
429B -> 441B -0.20192
430B -> 441B -0.15795
432B -> 441B 0.16932
433B -> 441B 0.24192
434B -> 441B -0.34498

Excited State 199: 1.000-A 3.4051 eV 364.12 nm f=0.0197 <S**2>=0.000
432A -> 441A 0.13812
432A -> 442A -0.12684
433A -> 442A 0.14235
435A -> 445A 0.53683
435A -> 447A 0.19861
436A -> 445A -0.10982
436A -> 447A 0.13074
436A -> 450A 0.10958
432B -> 441B 0.13813
432B -> 442B -0.12683
433B -> 442B 0.14235
435B -> 445B 0.53678
435B -> 447B 0.19861

| | |
|---|---|
| 436B -> 445B | -0.10981 |
| 436B -> 447B | 0.13074 |
| 436B -> 450B | 0.10960 |

Excited State 200: 3.000-A 3.4130 eV 363.27 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 430A -> 442A | 0.16319 |
| 431A -> 448A | -0.10204 |
| 432A -> 448A | -0.10510 |
| 433A -> 441A | -0.18311 |
| 434A -> 448A | 0.13026 |
| 435A -> 445A | -0.15712 |
| 435A -> 452A | 0.12577 |
| 436A -> 448A | -0.27951 |
| 436A -> 450A | 0.15681 |
| 436A -> 455A | -0.12187 |
| 436A -> 467A | 0.10385 |
| 430B -> 442B | -0.16319 |
| 431B -> 448B | 0.10204 |
| 432B -> 448B | 0.10510 |
| 433B -> 441B | 0.18312 |
| 434B -> 448B | -0.13026 |
| 435B -> 445B | 0.15719 |
| 435B -> 452B | -0.12577 |
| 436B -> 448B | 0.27951 |
| 436B -> 450B | -0.15680 |
| 436B -> 455B | 0.12186 |
| 436B -> 467B | -0.10385 |

**Table S9.** Standard orientation of the optimized geometry for the open-ring isomer (OF2) of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | -0.18024 | -2.14154 | -0.21421 |
| N | -4.46048 | -2.55754 | 0.14895 |
| C | -3.41173 | -1.94397 | -0.51338 |
| C | -3.9597 | -1.22071 | -1.65747 |
| C | -5.36079 | -1.44221 | -1.66196 |
| C | -5.79125 | -2.34473 | -0.47736 |
| C | -6.74106 | -1.60105 | 0.436099 |
| C | -8.02737 | -1.95941 | 0.589833 |
| C | -8.588 | -3.16357 | -0.05481 |
| C | -7.65047 | -3.9928 | -0.83741 |
| C | -6.36323 | -3.64517 | -1.00486 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O | -9.79383 | -3.47519 | 0.072178 | C | -5.80018 | 5.106876 | -3.76753 |
| C | -3.3761 | -0.46763 | -2.68178 | C | -5.66044 | 6.485595 | -3.57183 |
| C | -4.20336 | 0.058606 | -3.68426 | C | -4.7797 | 6.964553 | -2.59418 |
| C | -5.58839 | -0.1589 | -3.67762 | C | -4.04893 | 6.06877 | -1.80906 |
| C | -6.17903 | -0.91927 | -2.65482 | Cl | -0.23367 | 0.150683 | -1.64771 |
| C | -3.96517 | -3.40561 | 1.136753 | Cl | -0.07315 | -0.1901 | 1.645214 |
| C | -2.58365 | -3.27231 | 1.05803 | Ir | 0.199534 | 2.054527 | 0.196971 |
| N | -2.25309 | -2.34826 | 0.035624 | N | 4.078316 | -2.50568 | -0.44468 |
| C | -4.83165 | -4.2572 | 1.979145 | C | 2.980302 | -2.11671 | 0.300106 |
| C | -1.46792 | -3.96515 | 1.676591 | C | 3.402731 | -1.93055 | 1.685458 |
| C | -1.59301 | -4.89171 | 2.72688 | C | 4.78661 | -2.22455 | 1.741956 |
| C | -0.48035 | -5.61383 | 3.159835 | C | 5.350333 | -2.54587 | 0.335962 |
| C | 0.753347 | -5.42082 | 2.52689 | C | 5.972867 | -3.92338 | 0.300919 |
| C | 0.885903 | -4.47753 | 1.500448 | C | 7.285289 | -4.12063 | 0.090191 |
| C | -0.20379 | -3.69481 | 1.075824 | C | 8.20734 | -3.00445 | -0.20033 |
| C | -5.65377 | -3.69254 | 2.972049 | C | 7.616381 | -1.65444 | -0.26242 |
| C | -6.48546 | -4.50437 | 3.74991 | C | 6.305202 | -1.43542 | -0.05818 |
| C | -6.50106 | -5.8897 | 3.551965 | O | 9.430346 | -3.19758 | -0.39113 |
| C | -5.67882 | -6.46251 | 2.573772 | C | 2.70784 | -1.64486 | 2.865197 |
| C | -4.85159 | -5.65319 | 1.790518 | C | 3.412547 | -1.64436 | 4.075935 |
| N | -4.00137 | 2.946959 | -0.16512 | C | 4.783746 | -1.92858 | 4.121661 |
| C | -3.02761 | 2.216077 | 0.491191 | C | 5.485258 | -2.2202 | 2.941743 |
| C | -3.65346 | 1.545001 | 1.627767 | C | 3.65767 | -3.00433 | -1.68133 |
| C | -5.02099 | 1.92041 | 1.634309 | C | 2.271775 | -2.86508 | -1.66809 |
| C | -5.34998 | 2.87072 | 0.455139 | N | 1.873537 | -2.28671 | -0.44094 |
| C | -5.78684 | 4.220852 | 0.98633 | C | 4.57849 | -3.6249 | -2.65358 |
| C | -7.03007 | 4.700543 | 0.813554 | C | 1.178637 | -3.30738 | -2.52212 |
| C | -8.04385 | 3.976381 | 0.021098 | C | 1.331228 | -3.82991 | -3.81791 |
| C | -7.60692 | 2.724084 | -0.62709 | C | 0.224741 | -4.32827 | -4.50899 |
| C | -6.3655 | 2.233793 | -0.46841 | C | -1.03565 | -4.31261 | -3.89988 |
| O | -9.2098 | 4.41254 | -0.11029 | C | -1.19816 | -3.76552 | -2.62028 |
| C | -3.15858 | 0.71644 | 2.639935 | C | -0.11165 | -3.22122 | -1.91484 |
| C | -4.03974 | 0.274479 | 3.636962 | C | 5.651825 | -2.90308 | -3.20874 |
| C | -5.39077 | 0.648528 | 3.635821 | C | 6.540142 | -3.52179 | -4.094 |
| C | -5.89273 | 1.481418 | 2.622198 | C | 6.364552 | -4.8647 | -4.44635 |
| C | -3.4189 | 3.737601 | -1.15262 | C | 5.293774 | -5.58899 | -3.90773 |
| C | -2.06144 | 3.450498 | -1.07863 | C | 4.410166 | -4.97731 | -3.01495 |
| N | -1.83325 | 2.494998 | -0.05882 | N | 4.563354 | 1.764254 | 0.840705 |
| C | -4.18596 | 4.679142 | -1.99541 | C | 3.514047 | 1.671762 | -0.07168 |
| C | -0.87801 | 3.993222 | -1.71747 | C | 3.834066 | 1.430083 | -1.45388 |
| C | -0.8969 | 4.912293 | -2.78148 | C | 2.938454 | 0.777933 | -2.33135 |
| C | 0.297138 | 5.452446 | -3.25996 | C | 3.340139 | 0.362647 | -3.58919 |
| C | 1.51028 | 5.080454 | -2.66728 | C | 4.665149 | 0.586588 | -4.02625 |
| C | 1.530739 | 4.148548 | -1.62348 | C | 5.554088 | 1.264065 | -3.21046 |
| C | 0.350098 | 3.5598 | -1.14205 | C | 4.051867 | 2.234765 | 1.990602 |
| C | -5.06547 | 4.207908 | -2.98796 | C | 2.62114 | 2.383985 | 1.822468 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 2.299158 | 1.953665 | 0.541675 | H | -4.66495 | 8.032671 | -2.44107 |
| C | 4.940065 | 2.517135 | 3.131332 | H | -3.36415 | 6.438371 | -1.05276 |
| C | 1.561981 | 2.951025 | 2.597745 | H | 5.297214 | -4.75038 | 0.498014 |
| C | 1.666899 | 3.391853 | 3.940089 | H | 7.722793 | -5.11289 | 0.103665 |
| C | 0.616779 | 4.078696 | 4.530635 | H | 8.299915 | -0.84143 | -0.48308 |
| C | -0.54994 | 4.349404 | 3.786322 | H | 5.879058 | -0.43625 | -0.0792 |
| C | -0.69014 | 3.872563 | 2.484024 | H | 1.652437 | -1.41957 | 2.838757 |
| C | 0.329979 | 3.114322 | 1.87092 | H | 2.879501 | -1.42341 | 4.994401 |
| C | 5.936577 | 1.584482 | 3.479209 | H | 5.30645 | -1.92764 | 5.072184 |
| C | 6.840813 | 1.85919 | 4.507153 | H | 6.544715 | -2.45365 | 2.968327 |
| C | 6.778288 | 3.076663 | 5.196405 | H | 2.30956 | -3.8518 | -4.28458 |
| C | 5.808487 | 4.021714 | 4.842845 | H | 0.346769 | -4.73134 | -5.50944 |
| C | 4.898194 | 3.747094 | 3.818223 | H | -1.89649 | -4.71788 | -4.42495 |
| H | -6.32787 | -0.72929 | 0.93335 | H | -2.18709 | -3.75203 | -2.17728 |
| H | -8.70756 | -1.39037 | 1.214485 | H | 5.78326 | -1.85876 | -2.95161 |
| H | -8.05436 | -4.90717 | -1.25803 | H | 7.366804 | -2.95471 | -4.50987 |
| H | -5.67434 | -4.26187 | -1.57455 | H | 7.055113 | -5.34258 | -5.13369 |
| H | -2.31052 | -0.28741 | -2.69191 | H | 5.151919 | -6.6312 | -4.17521 |
| H | -3.75358 | 0.636971 | -4.48439 | H | 3.585361 | -5.54124 | -2.5922 |
| H | -6.20676 | 0.246793 | -4.47154 | H | 1.940913 | 0.548621 | -1.99269 |
| H | -7.24755 | -1.10958 | -2.65113 | H | 2.635756 | -0.16383 | -4.22376 |
| H | -2.55518 | -5.05445 | 3.198656 | H | 4.976736 | 0.255418 | -5.01143 |
| H | -0.57763 | -6.32823 | 3.971163 | H | 6.542883 | 1.507743 | -3.58245 |
| H | 1.618504 | -6.00041 | 2.837295 | H | 2.563457 | 3.184048 | 4.509141 |
| H | 1.854959 | -4.35273 | 1.035008 | H | 0.695513 | 4.412941 | 5.559853 |
| H | -5.62912 | -2.62051 | 3.136676 | H | -1.35545 | 4.919681 | 4.240621 |
| H | -7.11608 | -4.05732 | 4.511643 | H | -1.60785 | 4.071426 | 1.944856 |
| H | -7.14651 | -6.51842 | 4.156668 | H | 5.989097 | 0.648363 | 2.93727 |
| H | -5.68466 | -7.5365 | 2.418609 | H | 7.598289 | 1.126365 | 4.767162 |
| H | -4.21151 | -6.09579 | 1.034374 | H | 7.485435 | 3.291727 | 5.991085 |
| H | -5.04183 | 4.760274 | 1.563791 | H | 5.770052 | 4.97922 | 5.352376 |
| H | -7.3401 | 5.649577 | 1.237064 | H | 4.174606 | 4.500509 | 3.527689 |
| H | -8.33753 | 2.231135 | -1.25935 | C | 5.153828 | 1.772708 | -1.941 |
| H | -6.04194 | 1.326758 | -0.96868 | C | 6.033238 | 2.71129 | -1.27677 |
| H | -2.12089 | 0.41288 | 2.641667 | C | 7.462491 | 2.5441 | -1.35873 |
| H | -3.65939 | -0.36483 | 4.426532 | C | 5.543588 | 3.921068 | -0.66283 |
| H | -6.0507 | 0.305942 | 4.42607 | C | 8.323215 | 3.454189 | -0.81532 |
| H | -6.93337 | 1.789856 | 2.621707 | H | 7.851339 | 1.638741 | -1.81348 |
| H | -1.83771 | 5.206048 | -3.23204 | C | 6.3899 | 4.863791 | -0.15656 |
| H | 0.281526 | 6.161074 | -4.08182 | H | 4.475463 | 4.09831 | -0.65162 |
| H | 2.442667 | 5.510233 | -3.02232 | H | 9.397056 | 3.302986 | -0.82841 |
| H | 2.479838 | 3.864618 | -1.1928 | H | 6.018846 | 5.789849 | 0.267493 |
| H | -5.16083 | 3.139772 | -3.15173 | C | 7.836991 | 4.681008 | -0.18006 |
| H | -6.47611 | 4.732127 | -4.52931 | O | 8.637209 | 5.538298 | 0.299855 |
| H | -6.23081 | 7.181602 | -4.17825 | | | | |

Excited State 1: 3.000-A -0.5783 eV -2143.95 nm f=-0.0000 <S**2>=2.000

433A -> 438A 0.19938

434A -> 437A 0.27187

435A -> 438A -0.43687

436A -> 437A -0.43060

433B -> 438B -0.19939

434B -> 437B -0.27187

435B -> 438B 0.43687

436B -> 437B 0.43060

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -6023.98464200

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.000-A -0.5761 eV -2152.23 nm f=-0.0000 <S**2>=2.000

433A -> 437A 0.20952

434A -> 438A 0.25777

435A -> 437A -0.46285

436A -> 438A -0.40662

433B -> 437B -0.20952

434B -> 438B -0.25777

435B -> 437B 0.46286

436B -> 438B 0.40662

Excited State 3: 3.000-A 0.6694 eV 1852.18 nm f=0.0000 <S**2>=2.000

433A -> 438A -0.21407

434A -> 437A -0.23492

435A -> 438A 0.28790

436A -> 437A -0.55651

433B -> 438B 0.21408

434B -> 437B 0.23493

435B -> 438B -0.28796

436B -> 437B 0.55664

Excited State 4: 3.000-A 0.6835 eV 1814.05 nm f=0.0000 <S**2>=2.000

433A -> 437A -0.19517

434A -> 438A -0.16271

435A -> 437A 0.31452
436A -> 438A -0.57462
433B -> 437B 0.19517
434B -> 438B 0.16270
435B -> 437B -0.31462
436B -> 438B 0.57473

Excited State 5: 1.000-A 0.6979 eV 1776.52 nm f=0.0046 <S**2>=0.000
435A -> 438A -0.36422
436A -> 437A 0.60432
435B -> 438B -0.36417
436B -> 437B 0.60421

Excited State 6: 1.000-A 0.7042 eV 1760.65 nm f=0.0000 <S**2>=0.000
435A -> 437A 0.51104
436A -> 438A -0.48738
435B -> 437B 0.51099
436B -> 438B -0.48726

Excited State 7: 3.000-A 0.7633 eV 1624.27 nm f=0.0000 <S**2>=2.000
433A -> 437A 0.36458
434A -> 438A 0.40706
435A -> 437A 0.43102
433B -> 437B -0.36460
434B -> 438B -0.40707
435B -> 437B -0.43102

Excited State 8: 3.000-A 0.7691 eV 1612.05 nm f=0.0000 <S**2>=2.000
433A -> 438A -0.28822
434A -> 437A -0.41955
435A -> 438A -0.47231
433B -> 438B 0.28824
434B -> 437B 0.41957
435B -> 438B 0.47234

Excited State 9: 1.000-A 0.8626 eV 1437.30 nm f=0.0009 <S**2>=0.000

433A -> 438A 0.16666
434A -> 437A 0.35270
435A -> 438A 0.52432
436A -> 437A 0.28918
433B -> 438B 0.16663
434B -> 437B 0.35267
435B -> 438B 0.52429
436B -> 437B 0.28918

Excited State 10: 1.000-A 0.9084 eV 1364.85 nm f=0.1380 <S**2>=0.000
433A -> 437A 0.25119
434A -> 438A 0.30392
435A -> 437A 0.41179
436A -> 438A 0.43721
433B -> 437B 0.25117
434B -> 438B 0.30390
435B -> 437B 0.41178
436B -> 438B 0.43721
435A <- 437A -0.10368
436A <- 438A -0.10316
435B <- 437B -0.10368
436B <- 438B -0.10316

Excited State 11: 3.000-A 1.0815 eV 1146.42 nm f=0.0000 <S**2>=2.000
429A -> 438A 0.23006
430A -> 438A 0.22808
432A -> 437A -0.60681
429B -> 438B -0.23008
430B -> 438B -0.22810
432B -> 437B 0.60686

Excited State 12: 3.000-A 1.1002 eV 1126.89 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.26217
430A -> 437A 0.27290
432A -> 438A -0.57563
429B -> 437B -0.26219

430B -> 437B -0.27292
432B -> 438B 0.57567

Excited State 13: 3.000-A 1.1388 eV 1088.74 nm f=0.0000 <S**2>=2.000
433A -> 437A -0.51765
434A -> 438A 0.47019
433B -> 437B 0.52199
434B -> 438B -0.47331

Excited State 14: 1.000-A 1.1395 eV 1088.04 nm f=0.0000 <S**2>=0.000
433A -> 437A 0.57194
434A -> 438A -0.41145
433B -> 437B 0.56798
434B -> 438B -0.40786

Excited State 15: 1.000-A 1.1466 eV 1081.28 nm f=0.0103 <S**2>=0.000
432A -> 437A -0.29340
433A -> 438A -0.33680
434A -> 437A 0.49437
435A -> 438A -0.18372
436A -> 437A -0.11846
432B -> 437B -0.29288
433B -> 438B -0.34354
434B -> 437B 0.49941
435B -> 438B -0.18397
436B -> 437B -0.11812

Excited State 16: 3.000-A 1.1470 eV 1080.95 nm f=0.0000 <S**2>=2.000
433A -> 438A 0.56148
434A -> 437A -0.42164
433B -> 438B -0.55743
434B -> 437B 0.41565

Excited State 17: 1.000-A 1.1785 eV 1052.04 nm f=0.0059 <S**2>=0.000
429A -> 438A -0.11855
430A -> 438A -0.16921

432A -> 437A 0.47729
433A -> 438A -0.46124
429B -> 438B -0.11853
430B -> 438B -0.16918
432B -> 437B 0.47724
433B -> 438B -0.46118

Excited State 18: 1.000-A 1.1994 eV 1033.76 nm f=0.0487 <S**2>=0.000
429A -> 437A -0.18147
430A -> 437A -0.20765
432A -> 438A 0.51042
433A -> 437A -0.15121
434A -> 438A -0.28468
435A -> 437A 0.18459
436A -> 438A 0.18287
429B -> 437B -0.18145
430B -> 437B -0.20763
432B -> 438B 0.51038
433B -> 437B -0.15121
434B -> 438B -0.28468
435B -> 437B 0.18459
436B -> 438B 0.18287

Excited State 19: 3.000-A 1.2048 eV 1029.06 nm f=0.0000 <S**2>=2.000
424A -> 437A -0.19333
424A -> 438A 0.15532
425A -> 437A -0.47020
425A -> 438A 0.44083
424B -> 437B 0.19259
424B -> 438B -0.15464
425B -> 437B 0.47048
425B -> 438B -0.44109

Excited State 20: 3.000-A 1.2054 eV 1028.53 nm f=0.0000 <S**2>=2.000
424A -> 437A -0.46959
424A -> 438A -0.44293

425A -> 437A 0.19066
425A -> 438A 0.15415
424B -> 437B 0.46988
424B -> 438B 0.44313
425B -> 437B -0.18992
425B -> 438B -0.15344

Excited State 21: 1.000-A 1.3876 eV 893.54 nm f=0.0789 <S**2>=0.000
431A -> 437A -0.11303
432A -> 437A 0.38407
433A -> 438A 0.35179
434A -> 437A 0.34444
435A -> 438A -0.24758
436A -> 437A -0.20939
431B -> 437B -0.11304
432B -> 437B 0.38407
433B -> 438B 0.35179
434B -> 437B 0.34445
435B -> 438B -0.24758
436B -> 437B -0.20938
435A <- 438A 0.11796
436A <- 437A 0.11123
435B <- 438B 0.11796
436B <- 437B 0.11123

Excited State 22: 1.000-A 1.4012 eV 884.86 nm f=0.1240 <S**2>=0.000
430A -> 437A -0.10267
432A -> 438A 0.40712
433A -> 437A 0.27676
434A -> 438A 0.38059
435A -> 437A -0.22536
436A -> 438A -0.21943
430B -> 437B -0.10267
432B -> 438B 0.40712
433B -> 437B 0.27676
434B -> 438B 0.38060

435B -> 437B -0.22536
436B -> 438B -0.21943
435A <- 437A 0.11966
436A <- 438A 0.10667
435B <- 437B 0.11966
436B <- 438B 0.10667

Excited State 23: 3.000-A 1.4439 eV 858.68 nm f=0.0000 <S**2>=2.000
428A -> 437A 0.10496
430A -> 437A -0.55713
431A -> 438A -0.27619
432A -> 438A -0.26534
433A -> 437A 0.10518
428B -> 437B -0.10498
430B -> 437B 0.55724
431B -> 438B 0.27622
432B -> 438B 0.26539
433B -> 437B -0.10519

Excited State 24: 3.000-A 1.4535 eV 853.00 nm f=0.0000 <S**2>=2.000
430A -> 438A -0.46015
431A -> 437A -0.46480
432A -> 437A -0.15951
433A -> 438A 0.12134
430B -> 438B 0.46023
431B -> 437B 0.46486
432B -> 437B 0.15954
433B -> 438B -0.12134

Excited State 25: 1.000-A 1.4763 eV 839.80 nm f=0.0009 <S**2>=0.000
429A -> 437A 0.12019
430A -> 437A 0.60599
431A -> 438A 0.17866
432A -> 438A 0.26013
429B -> 437B 0.12022
430B -> 437B 0.60589

431B -> 438B 0.17859
432B -> 438B 0.26010

Excited State 26: 1.000-A 1.4954 eV 829.10 nm f=0.0000 <S**2>=0.000
430A -> 438A 0.52372
431A -> 437A 0.42272
432A -> 437A 0.17641
430B -> 438B 0.52371
431B -> 437B 0.42259
432B -> 437B 0.17645

Excited State 27: 3.000-A 1.5013 eV 825.83 nm f=0.0000 <S**2>=2.000
429A -> 438A -0.41517
430A -> 438A -0.28920
431A -> 437A 0.35499
432A -> 437A -0.29905
429B -> 438B 0.41518
430B -> 438B 0.28912
431B -> 437B -0.35511
432B -> 437B 0.29901

Excited State 28: 3.000-A 1.5029 eV 824.99 nm f=0.0000 <S**2>=2.000
429A -> 437A -0.50950
431A -> 438A 0.35625
432A -> 438A -0.29316
429B -> 437B 0.50953
431B -> 438B -0.35629
432B -> 438B 0.29314

Excited State 29: 1.000-A 1.5625 eV 793.48 nm f=0.0077 <S**2>=0.000
424A -> 437A 0.18199
425A -> 438A -0.16724
428A -> 438A 0.11512
429A -> 438A -0.29293
430A -> 438A -0.29150
431A -> 437A 0.46023

424B -> 437B 0.18186
425B -> 438B -0.16714
428B -> 438B 0.11513
429B -> 438B -0.29289
430B -> 438B -0.29149
431B -> 437B 0.46021

Excited State 30: 1.000-A 1.5691 eV 790.16 nm f=0.0092 <S**2>=0.000
424A -> 437A -0.12111
424A -> 438A -0.24328
425A -> 437A 0.26868
425A -> 438A -0.10852
429A -> 437A 0.44031
431A -> 438A -0.36203
424B -> 437B -0.12154
424B -> 438B -0.24311
425B -> 437B 0.26849
425B -> 438B -0.10891
429B -> 437B 0.44027
431B -> 438B -0.36199

Excited State 31: 1.000-A 1.5880 eV 780.74 nm f=0.0056 <S**2>=0.000
424A -> 437A 0.42410
424A -> 438A 0.15658
425A -> 437A 0.21630
425A -> 438A -0.39521
430A -> 438A 0.13192
431A -> 437A -0.20582
424B -> 437B 0.42378
424B -> 438B 0.15719
425B -> 437B 0.21694
425B -> 438B -0.39498
430B -> 438B 0.13192
431B -> 437B -0.20584

Excited State 32: 1.659-A 1.5923 eV 778.66 nm f=0.0147 <S**2>=0.438

424A -> 437A -0.17432
424A -> 438A -0.31282
425A -> 437A 0.32871
425A -> 438A -0.11624
427A -> 438A -0.11459
428A -> 437A -0.19772
429A -> 437A -0.32233
424B -> 437B -0.17663
424B -> 438B -0.31752
425B -> 437B 0.33255
425B -> 438B -0.11898
427B -> 438B 0.14157
428B -> 437B 0.29792
429B -> 437B -0.13987
431B -> 438B 0.38667

Excited State 33: 2.692-A 1.5923 eV 778.66 nm f=0.0041 <S**2>=1.562
424A -> 438A -0.17162
425A -> 437A 0.17908
427A -> 438A 0.24892
428A -> 437A 0.49432
431A -> 438A 0.40088
424B -> 438B -0.16233
425B -> 437B 0.17116
427B -> 438B -0.23468
428B -> 437B -0.44137
429B -> 437B -0.29466
431B -> 438B -0.14428

Excited State 34: 3.000-A 1.6023 eV 773.78 nm f=0.0000 <S**2>=2.000
427A -> 437A -0.32120
428A -> 438A -0.46481
429A -> 438A -0.32602
431A -> 437A -0.23061
427B -> 437B 0.32124
428B -> 438B 0.46487

429B -> 438B 0.32610
431B -> 437B 0.23059

Excited State 35: 1.000-A 1.6241 eV 763.42 nm f=0.0092 <S**2>=0.000
427A -> 438A 0.19891
428A -> 437A 0.45335
429A -> 437A 0.32586
430A -> 437A -0.10158
431A -> 438A 0.35127
427B -> 438B 0.19885
428B -> 437B 0.45322
429B -> 437B 0.32581
430B -> 437B -0.10158
431B -> 438B 0.35121

Excited State 36: 1.000-A 1.6484 eV 752.15 nm f=0.0118 <S**2>=0.000
427A -> 437A 0.25260
428A -> 438A 0.39009
429A -> 438A 0.49023
430A -> 438A -0.10131
431A -> 437A 0.10604
427B -> 437B 0.25255
428B -> 438B 0.39002
429B -> 438B 0.49017
430B -> 438B -0.10130
431B -> 437B 0.10600

Excited State 37: 3.000-A 1.6679 eV 743.34 nm f=0.0000 <S**2>=2.000
427A -> 438A 0.18197
428A -> 437A 0.29108
429A -> 437A -0.32219
430A -> 437A 0.30447
431A -> 438A -0.42442
427B -> 438B -0.18207
428B -> 437B -0.29129
429B -> 437B 0.32232

430B -> 437B -0.30459
431B -> 438B 0.42459

Excited State 38: 1.000-A 1.6799 eV 738.03 nm f=0.0004 <S**2>=0.000
427A -> 438A 0.20840
428A -> 437A 0.43557
429A -> 437A -0.27589
430A -> 437A 0.24672
431A -> 438A -0.35558
427B -> 438B 0.20831
428B -> 437B 0.43542
429B -> 437B -0.27574
430B -> 437B 0.24656
431B -> 438B -0.35540

Excited State 39: 3.000-A 1.6835 eV 736.45 nm f=0.0000 <S**2>=2.000
427A -> 437A 0.25414
428A -> 438A 0.28766
429A -> 438A -0.36390
430A -> 438A 0.35816
431A -> 437A -0.29074
427B -> 437B -0.25423
428B -> 438B -0.28776
429B -> 438B 0.36401
430B -> 438B -0.35825
431B -> 437B 0.29078

Excited State 40: 1.000-A 1.7049 eV 727.24 nm f=0.0000 <S**2>=0.000
427A -> 437A 0.30273
428A -> 438A 0.39187
429A -> 438A -0.36690
430A -> 438A 0.28031
431A -> 437A -0.19447
427B -> 437B 0.30265
428B -> 438B 0.39178
429B -> 438B -0.36680

430B -> 438B 0.28022
431B -> 437B -0.19439

Excited State 41: 3.000-A 1.8453 eV 671.89 nm f=0.0000 <S**2>=2.000
410A -> 437A 0.11557
420A -> 438A -0.10119
421A -> 437A -0.21786
422A -> 438A 0.15446
423A -> 438A -0.12006
426A -> 437A -0.15065
427A -> 437A -0.44442
428A -> 438A 0.33447
429A -> 438A -0.10807
410B -> 437B -0.11557
420B -> 438B 0.10120
421B -> 437B 0.21787
422B -> 438B -0.15446
423B -> 438B 0.12007
426B -> 437B 0.15066
427B -> 437B 0.44452
428B -> 438B -0.33455
429B -> 438B 0.10807

Excited State 42: 3.000-A 1.8560 eV 668.03 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.11656
410A -> 438A 0.13488
416A -> 437A 0.11834
420A -> 437A -0.13659
421A -> 438A -0.23079
422A -> 437A 0.19792
423A -> 437A -0.14025
426A -> 438A -0.13204
427A -> 438A -0.43821
428A -> 437A 0.23139
429A -> 437A -0.10263
409B -> 437B 0.11656

410B -> 438B -0.13488
416B -> 437B -0.11833
420B -> 437B 0.13660
421B -> 438B 0.23080
422B -> 437B -0.19793
423B -> 437B 0.14026
426B -> 438B 0.13204
427B -> 438B 0.43829
428B -> 437B -0.23143
429B -> 437B 0.10263

Excited State 43: 1.000-A 1.8720 eV 662.33 nm f=0.0014 <S**2>=0.000
427A -> 437A 0.57087
428A -> 438A -0.40921
427B -> 437B 0.57087
428B -> 438B -0.40922

Excited State 44: 3.000-A 1.8857 eV 657.51 nm f=0.0000 <S**2>=2.000
409A -> 438A -0.12523
410A -> 437A 0.18593
416A -> 438A 0.19842
417A -> 437A 0.13009
421A -> 437A -0.27017
422A -> 438A 0.13816
423A -> 438A -0.11895
426A -> 437A -0.19690
427A -> 437A 0.31694
428A -> 438A -0.26918
409B -> 438B 0.12523
410B -> 437B -0.18592
416B -> 438B -0.19841
417B -> 437B -0.13009
421B -> 437B 0.27017
422B -> 438B -0.13817
423B -> 438B 0.11896
426B -> 437B 0.19691

427B -> 437B -0.31679
428B -> 438B 0.26907

Excited State 45: 3.000-A 1.8922 eV 655.25 nm f=0.0000 <S**2>=2.000
409A -> 437A 0.12856
410A -> 438A -0.16936
416A -> 437A -0.21625
417A -> 438A -0.12583
419A -> 437A 0.10260
421A -> 438A 0.22085
422A -> 437A -0.12749
426A -> 438A 0.11200
427A -> 438A -0.40324
428A -> 437A 0.25429
409B -> 437B -0.12861
410B -> 438B 0.16940
416B -> 437B 0.21656
417B -> 438B 0.12584
419B -> 437B -0.10243
421B -> 438B -0.22062
422B -> 437B 0.12697
426B -> 438B -0.11224
427B -> 438B 0.41145
428B -> 437B -0.25815

Excited State 46: 1.000-A 1.8925 eV 655.14 nm f=0.0002 <S**2>=0.000
427A -> 438A 0.63738
428A -> 437A -0.29966
427B -> 438B 0.63206
428B -> 437B -0.29633

Excited State 47: 3.000-A 1.9267 eV 643.50 nm f=0.0000 <S**2>=2.000
434A -> 439A -0.11191
435A -> 440A -0.22147
436A -> 439A -0.65571
434B -> 439B 0.11192

435B -> 440B 0.22149
436B -> 439B 0.65579

Excited State 48: 3.000-A 1.9297 eV 642.51 nm f=0.0000 <S**2>=2.000
410A -> 437A -0.11677
416A -> 438A -0.11419
417A -> 437A -0.10803
420A -> 438A 0.10538
421A -> 437A 0.12382
423A -> 438A -0.26457
426A -> 437A -0.55679
410B -> 437B 0.11677
416B -> 438B 0.11419
417B -> 437B 0.10803
420B -> 438B -0.10538
421B -> 437B -0.12382
423B -> 438B 0.26459
426B -> 437B 0.55684

Excited State 49: 1.000-A 1.9305 eV 642.25 nm f=0.0000 <S**2>=0.000
434A -> 439A 0.10779
435A -> 440A 0.21641
436A -> 439A 0.65987
434B -> 439B 0.10777
435B -> 440B 0.21639
436B -> 439B 0.65980

Excited State 50: 3.000-A 1.9480 eV 636.49 nm f=0.0000 <S**2>=2.000
416A -> 437A -0.10078
419A -> 437A 0.10874
423A -> 437A -0.36466
426A -> 438A -0.51886
416B -> 437B 0.10078
419B -> 437B -0.10874
423B -> 437B 0.36469
426B -> 438B 0.51889

Excited State 51: 3.000-A 1.9526 eV 634.98 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 433A -> 439A | -0.10920 |
| 435A -> 439A | -0.49864 |
| 436A -> 440A | -0.47663 |
| 433B -> 439B | 0.10921 |
| 435B -> 439B | 0.49868 |
| 436B -> 440B | 0.47667 |

Excited State 52: 1.000-A 1.9567 eV 633.62 nm f=0.0000 <S**2>=0.000

| | |
|---|---|
| 433A -> 439A | 0.10414 |
| 435A -> 439A | 0.50121 |
| 436A -> 440A | 0.47759 |
| 433B -> 439B | 0.10413 |
| 435B -> 439B | 0.50117 |
| 436B -> 440B | 0.47755 |

Excited State 53: 1.000-A 2.0096 eV 616.95 nm f=0.0023 <S**2>=0.000

| | |
|---|---|
| 423A -> 438A | 0.24603 |
| 426A -> 437A | 0.65767 |
| 423B -> 438B | 0.24601 |
| 426B -> 437B | 0.65762 |

Excited State 54: 3.000-A 2.0365 eV 608.80 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 435A -> 439A | 0.48802 |
| 436A -> 440A | -0.50625 |
| 435B -> 439B | -0.48843 |
| 436B -> 440B | 0.50667 |

Excited State 55: 1.000-A 2.0368 eV 608.72 nm f=0.0000 <S**2>=0.000

| | |
|---|---|
| 435A -> 439A | -0.48772 |
| 436A -> 440A | 0.50753 |
| 435B -> 439B | -0.48731 |
| 436B -> 440B | 0.50711 |

Excited State 56: 1.000-A 2.0465 eV 605.84 nm f=0.0266 <S**2>=0.000

423A -> 437A 0.40579
426A -> 438A 0.57295
423B -> 437B 0.40577
426B -> 438B 0.57293

Excited State 57: 3.000-A 2.0625 eV 601.14 nm f=0.0000 <S**2>=2.000
435A -> 440A -0.66109
436A -> 439A 0.23395
435B -> 440B 0.66119
436B -> 439B -0.23399

Excited State 58: 1.000-A 2.0632 eV 600.92 nm f=0.0001 <S**2>=0.000
435A -> 440A 0.66410
436A -> 439A -0.22703
435B -> 440B 0.66399
436B -> 439B -0.22699

Excited State 59: 3.000-A 2.0678 eV 599.60 nm f=0.0000 <S**2>=2.000
411A -> 437A 0.23696
412A -> 437A 0.22291
413A -> 438A -0.30852
414A -> 438A -0.15179
415A -> 437A -0.14382
417A -> 438A 0.23038
419A -> 437A -0.34930
423A -> 437A -0.10250
426A -> 438A -0.10084
411B -> 437B -0.23696
412B -> 437B -0.22291
413B -> 438B 0.30853
414B -> 438B 0.15178
415B -> 437B 0.14382
417B -> 438B -0.23038
419B -> 437B 0.34930
423B -> 437B 0.10247
426B -> 438B 0.10079

Excited State 60: 3.000-A 2.0711 eV 598.63 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 411A -> 438A | 0.21677 |
| 412A -> 438A | 0.20169 |
| 413A -> 437A | -0.34808 |
| 414A -> 437A | -0.17429 |
| 415A -> 438A | -0.13974 |
| 417A -> 437A | 0.26891 |
| 419A -> 438A | -0.31057 |
| 426A -> 437A | -0.10256 |
| 411B -> 438B | -0.21678 |
| 412B -> 438B | -0.20169 |
| 413B -> 437B | 0.34809 |
| 414B -> 437B | 0.17428 |
| 415B -> 438B | 0.13974 |
| 417B -> 437B | -0.26891 |
| 419B -> 438B | 0.31057 |
| 426B -> 437B | 0.10254 |

Excited State 61: 3.000-A 2.1767 eV 569.60 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 422A -> 437A | -0.22937 |
| 423A -> 437A | -0.51421 |
| 426A -> 438A | 0.35191 |
| 422B -> 437B | 0.22943 |
| 423B -> 437B | 0.51449 |
| 426B -> 438B | -0.35211 |

Excited State 62: 1.000-A 2.1883 eV 566.58 nm f=0.0006 <S**2>=0.000

| | |
|---|---|
| 420A -> 437A | 0.12347 |
| 423A -> 437A | 0.55760 |
| 426A -> 438A | -0.39624 |
| 420B -> 437B | 0.12343 |
| 423B -> 437B | 0.55736 |
| 426B -> 438B | -0.39608 |

Excited State 63: 3.000-A 2.1968 eV 564.40 nm f=0.0000 <S**2>=2.000

413A -> 437A 0.11994
417A -> 437A 0.13627
421A -> 437A 0.13822
422A -> 438A -0.21526
423A -> 438A -0.54634
426A -> 437A 0.25528
413B -> 437B -0.11994
417B -> 437B -0.13628
421B -> 437B -0.13824
422B -> 438B 0.21529
423B -> 438B 0.54648
426B -> 437B -0.25533

Excited State 64: 3.000-A 2.2206 eV 558.35 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.11733
410A -> 438A 0.16457
412A -> 437A -0.12132
413A -> 438A 0.14437
415A -> 437A -0.16038
416A -> 437A 0.16200
418A -> 438A -0.15479
421A -> 438A 0.24153
422A -> 437A -0.40524
423A -> 437A 0.17113
426A -> 438A -0.19914
409B -> 437B 0.11733
410B -> 438B -0.16457
412B -> 437B 0.12132
413B -> 438B -0.14437
415B -> 437B 0.16039
416B -> 437B -0.16200
418B -> 438B 0.15480
421B -> 438B -0.24157
422B -> 437B 0.40531
423B -> 437B -0.17111
426B -> 438B 0.19913

Excited State 65: 1.000-A 2.2221 eV 557.97 nm f=0.0002 <S**2>=0.000

| | |
|---|---|
| 420A -> 438A | 0.10037 |
| 423A -> 438A | 0.64483 |
| 426A -> 437A | -0.23928 |
| 420B -> 438B | 0.10040 |
| 423B -> 438B | 0.64482 |
| 426B -> 437B | -0.23931 |

Excited State 66: 3.000-A 2.2258 eV 557.04 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 409A -> 438A | 0.13501 |
| 410A -> 437A | -0.22171 |
| 412A -> 438A | 0.10374 |
| 413A -> 437A | -0.14405 |
| 415A -> 438A | 0.16993 |
| 416A -> 438A | -0.13163 |
| 418A -> 437A | 0.18535 |
| 421A -> 437A | -0.32543 |
| 422A -> 438A | 0.28534 |
| 423A -> 438A | -0.22197 |
| 426A -> 437A | 0.17200 |
| 409B -> 438B | -0.13501 |
| 410B -> 437B | 0.22171 |
| 412B -> 438B | -0.10374 |
| 413B -> 437B | 0.14405 |
| 415B -> 438B | -0.16993 |
| 416B -> 438B | 0.13163 |
| 418B -> 437B | -0.18536 |
| 421B -> 437B | 0.32552 |
| 422B -> 438B | -0.28542 |
| 423B -> 438B | 0.22167 |
| 426B -> 437B | -0.17190 |

Excited State 67: 1.000-A 2.2614 eV 548.25 nm f=0.0136 <S**2>=0.000

| | |
|---|---|
| 420A -> 438A | 0.14150 |
| 421A -> 437A | 0.57849 |

422A -> 438A -0.33725
420B -> 438B 0.14149
421B -> 437B 0.57844
422B -> 438B -0.33720

Excited State 68: 1.000-A 2.2675 eV 546.78 nm f=0.0687 <S**2>=0.000
420A -> 437A -0.12009
421A -> 438A -0.38265
422A -> 437A 0.55760
420B -> 437B -0.12008
421B -> 438B -0.38261
422B -> 437B 0.55755

Excited State 69: 3.000-A 2.2835 eV 542.96 nm f=0.0000 <S**2>=2.000
410A -> 437A -0.12324
417A -> 437A 0.14232
424A -> 437A -0.38072
424A -> 438A 0.15408
425A -> 437A -0.21260
425A -> 438A -0.44502
410B -> 437B 0.12324
417B -> 437B -0.14233
424B -> 437B 0.38043
424B -> 438B -0.15431
425B -> 437B 0.21390
425B -> 438B 0.44539

Excited State 70: 3.000-A 2.2847 eV 542.66 nm f=0.0000 <S**2>=2.000
424A -> 437A -0.22181
424A -> 438A 0.47123
425A -> 437A 0.40441
425A -> 438A 0.17088
424B -> 437B 0.22162
424B -> 438B -0.47099
425B -> 437B -0.40499
425B -> 438B -0.17294

Excited State 71: 1.000-A 2.2861 eV 542.33 nm f=0.0000 <S**2>=0.000

| | |
|---|---|
| 424A -> 437A | 0.13364 |
| 424A -> 438A | 0.22539 |
| 425A -> 437A | 0.44984 |
| 425A -> 438A | 0.47361 |
| 424B -> 437B | 0.13295 |
| 424B -> 438B | 0.22376 |
| 425B -> 437B | 0.44882 |
| 425B -> 438B | 0.47293 |

Excited State 72: 1.000-A 2.2864 eV 542.27 nm f=0.0000 <S**2>=0.000

| | |
|---|---|
| 424A -> 437A | -0.45193 |
| 424A -> 438A | 0.47290 |
| 425A -> 437A | 0.13086 |
| 425A -> 438A | -0.21954 |
| 424B -> 437B | -0.45246 |
| 424B -> 438B | 0.47380 |
| 425B -> 437B | 0.13052 |
| 425B -> 438B | -0.21875 |

Excited State 73: 3.000-A 2.2962 eV 539.94 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 409A -> 438A | -0.20452 |
| 410A -> 437A | 0.25780 |
| 412A -> 438A | 0.10001 |
| 413A -> 437A | -0.17957 |
| 415A -> 438A | -0.10922 |
| 416A -> 438A | -0.12264 |
| 417A -> 437A | -0.29751 |
| 419A -> 438A | 0.12745 |
| 421A -> 437A | 0.13925 |
| 422A -> 438A | 0.13535 |
| 423A -> 438A | -0.18667 |
| 424A -> 437A | -0.18505 |
| 425A -> 438A | -0.18958 |
| 409B -> 438B | 0.20453 |

410B -> 437B -0.25780
412B -> 438B -0.10001
413B -> 437B 0.17958
415B -> 438B 0.10922
416B -> 438B 0.12264
417B -> 437B 0.29753
419B -> 438B -0.12746
421B -> 437B -0.13925
422B -> 438B -0.13537
423B -> 438B 0.18666
424B -> 437B 0.18493
425B -> 438B 0.18938

Excited State 74: 3.000-A 2.3008 eV 538.87 nm f=0.0000 <S**2>=2.000
397A -> 437A -0.10233
406A -> 437A 0.12002
409A -> 437A -0.25451
410A -> 438A 0.25769
412A -> 437A 0.11807
413A -> 438A -0.15894
415A -> 437A -0.17396
416A -> 437A -0.13582
417A -> 438A -0.26119
419A -> 437A 0.18388
421A -> 438A 0.19050
422A -> 437A 0.11773
423A -> 437A -0.13936
424A -> 438A -0.11796
425A -> 437A -0.10803
397B -> 437B 0.10233
406B -> 437B -0.12002
409B -> 437B 0.25451
410B -> 438B -0.25769
412B -> 437B -0.11807
413B -> 438B 0.15894
415B -> 437B 0.17396

416B -> 437B 0.13583
417B -> 438B 0.26120
419B -> 437B -0.18390
421B -> 438B -0.19051
422B -> 437B -0.11774
423B -> 437B 0.13936
424B -> 438B 0.11788
425B -> 437B 0.10793

Excited State 75: 1.000-A 2.3333 eV 531.36 nm f=0.0042 <S**2>=0.000
413A -> 438A 0.12016
416A -> 437A 0.13179
417A -> 438A -0.11583
418A -> 438A -0.21798
419A -> 437A 0.41771
420A -> 437A -0.28149
421A -> 438A -0.23033
422A -> 437A -0.25038
413B -> 438B 0.12007
416B -> 437B 0.13182
417B -> 438B -0.11588
418B -> 438B -0.21805
419B -> 437B 0.41785
420B -> 437B -0.28172
421B -> 438B -0.23049
422B -> 437B -0.25056

Excited State 76: 3.000-A 2.3401 eV 529.81 nm f=0.0000 <S**2>=2.000
396A -> 438A 0.17211
397A -> 437A 0.18612
411A -> 437A -0.11212
413A -> 438A 0.13416
418A -> 438A 0.12184
419A -> 437A -0.22278
420A -> 437A 0.36608
421A -> 438A 0.25265

422A -> 437A 0.28695
396B -> 438B -0.17209
397B -> 437B -0.18610
411B -> 437B 0.11217
413B -> 438B -0.13424
418B -> 438B -0.12169
419B -> 437B 0.22249
420B -> 437B -0.36594
421B -> 438B -0.25253
422B -> 437B -0.28681

Excited State 77: 3.000-A 2.3454 eV 528.63 nm f=0.0000 <S**2>=2.000
431A -> 439A -0.13857
433A -> 440A 0.26797
434A -> 439A 0.61092
436A -> 439A -0.11872
431B -> 439B 0.13856
433B -> 440B -0.26793
434B -> 439B -0.61082
436B -> 439B 0.11870

Excited State 78: 3.000-A 2.3476 eV 528.14 nm f=0.0000 <S**2>=2.000
396A -> 437A -0.22804
397A -> 438A -0.21648
413A -> 437A -0.12449
416A -> 438A 0.10849
418A -> 437A -0.31443
419A -> 438A 0.28325
420A -> 438A -0.14244
421A -> 437A -0.23052
422A -> 438A -0.23225
396B -> 437B 0.22805
397B -> 438B 0.21649
413B -> 437B 0.12445
416B -> 438B -0.10854
418B -> 437B 0.31456

419B -> 438B -0.28338
420B -> 438B 0.14248
421B -> 437B 0.23056
422B -> 438B 0.23239

Excited State 79: 1.000-A 2.3524 eV 527.06 nm f=0.0002 <S**2>=0.000
431A -> 439A -0.12515
433A -> 440A 0.26184
434A -> 439A 0.62306
436A -> 439A -0.11233
431B -> 439B -0.12518
433B -> 440B 0.26188
434B -> 439B 0.62315
436B -> 439B -0.11235

Excited State 80: 1.000-A 2.3577 eV 525.86 nm f=0.0131 <S**2>=0.000
413A -> 437A 0.13926
416A -> 438A 0.13625
417A -> 437A -0.15554
418A -> 437A -0.34934
419A -> 438A 0.36457
420A -> 438A -0.12281
421A -> 437A -0.10245
422A -> 438A -0.34566
413B -> 437B 0.13930
416B -> 438B 0.13621
417B -> 437B -0.15552
418B -> 437B -0.34921
419B -> 438B 0.36446
420B -> 438B -0.12277
421B -> 437B -0.10238
422B -> 438B -0.34558

Excited State 81: 3.000-A 2.3609 eV 525.15 nm f=0.0000 <S**2>=2.000
431A -> 440A -0.12366
433A -> 439A 0.51921

434A -> 440A 0.41175
435A -> 439A -0.10144
436A -> 440A -0.11323
431B -> 440B 0.12365
433B -> 439B -0.51915
434B -> 440B -0.41170
435B -> 439B 0.10143
436B -> 440B 0.11321

Excited State 82: 3.000-A 2.3646 eV 524.33 nm f=0.0000 <S**2>=2.000
396A -> 438A 0.14629
397A -> 437A 0.17929
409A -> 437A -0.13404
416A -> 437A -0.23576
417A -> 438A -0.12922
418A -> 438A 0.30434
419A -> 437A -0.25557
420A -> 437A -0.32387
422A -> 437A -0.22510
396B -> 438B -0.14630
397B -> 437B -0.17931
409B -> 437B 0.13403
416B -> 437B 0.23580
417B -> 438B 0.12920
418B -> 438B -0.30445
419B -> 437B 0.25573
420B -> 437B 0.32405
422B -> 437B 0.22520

Excited State 83: 1.000-A 2.3692 eV 523.32 nm f=0.0001 <S**2>=0.000
431A -> 440A -0.11202
433A -> 439A 0.52434
434A -> 440A 0.41990
436A -> 440A -0.10718
431B -> 440B -0.11204
433B -> 439B 0.52440

434B -> 440B 0.41994
436B -> 440B -0.10719

Excited State 84: 1.000-A 2.3741 eV 522.23 nm f=0.0036 <S**2>=0.000
418A -> 438A -0.21502
419A -> 437A 0.35591
420A -> 437A 0.35991
421A -> 438A 0.29225
422A -> 437A 0.25347
418B -> 438B -0.21489
419B -> 437B 0.35580
420B -> 437B 0.35973
421B -> 438B 0.29221
422B -> 437B 0.25334

Excited State 85: 3.000-A 2.3808 eV 520.76 nm f=0.0000 <S**2>=2.000
416A -> 438A -0.12469
417A -> 437A -0.13829
418A -> 437A 0.28999
419A -> 438A -0.14351
420A -> 438A -0.32040
421A -> 437A -0.15415
422A -> 438A -0.43919
416B -> 438B 0.12472
417B -> 437B 0.13826
418B -> 437B -0.29012
419B -> 438B 0.14362
420B -> 438B 0.32047
421B -> 437B 0.15427
422B -> 438B 0.43938

Excited State 86: 1.000-A 2.3913 eV 518.48 nm f=0.0119 <S**2>=0.000
418A -> 437A -0.26641
419A -> 438A 0.23414
420A -> 438A 0.11753
421A -> 437A 0.29623

422A -> 438A 0.49167
418B -> 437B -0.26629
419B -> 438B 0.23408
420B -> 438B 0.11738
421B -> 437B 0.29616
422B -> 438B 0.49147

Excited State 87: 1.000-A 2.4213 eV 512.05 nm f=0.0002 <S**2>=0.000
416A -> 437A 0.12365
420A -> 437A 0.49495
421A -> 438A -0.41459
422A -> 437A -0.19462
416B -> 437B 0.12363
420B -> 437B 0.49521
421B -> 438B -0.41483
422B -> 437B -0.19478

Excited State 88: 3.000-A 2.4288 eV 510.48 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.10930
417A -> 438A -0.13492
418A -> 438A 0.17063
420A -> 437A 0.43590
421A -> 438A -0.37674
422A -> 437A -0.24585
409B -> 437B 0.10932
417B -> 438B 0.13496
418B -> 438B -0.17062
420B -> 437B -0.43559
421B -> 438B 0.37648
422B -> 437B 0.24573

Excited State 89: 3.000-A 2.4450 eV 507.09 nm f=0.0000 <S**2>=2.000
396A -> 437A 0.10554
397A -> 438A 0.10172
418A -> 437A -0.16446
420A -> 438A -0.54790

421A -> 437A 0.25490
422A -> 438A 0.18332
396B -> 437B -0.10554
397B -> 438B -0.10173
418B -> 437B 0.16444
420B -> 438B 0.54817
421B -> 437B -0.25497
422B -> 438B -0.18334

Excited State 90: 1.000-A 2.4554 eV 504.95 nm f=0.0006 <S**2>=0.000
416A -> 438A 0.10063
417A -> 437A 0.12112
420A -> 438A 0.64048
421A -> 437A -0.18828
416B -> 438B 0.10061
417B -> 437B 0.12097
420B -> 438B 0.64057
421B -> 437B -0.18862

Excited State 91: 3.000-A 2.4559 eV 504.85 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.13304
396A -> 437A -0.33461
397A -> 438A -0.32534
399A -> 438A 0.11073
412A -> 438A -0.10527
413A -> 437A 0.12656
414A -> 437A 0.11942
415A -> 438A 0.13374
418A -> 437A 0.24926
419A -> 438A -0.13466
420A -> 438A -0.13577
421A -> 437A 0.17755
395B -> 437B 0.13309
396B -> 437B 0.33463
397B -> 438B 0.32536
399B -> 438B -0.11074

412B -> 438B 0.10540
413B -> 437B -0.12670
414B -> 437B -0.11940
415B -> 438B -0.13383
418B -> 437B -0.24911
419B -> 438B 0.13459
420B -> 438B 0.13421
421B -> 437B -0.17709

Excited State 92: 3.000-A 2.4606 eV 503.87 nm f=0.0000 <S**2>=2.000
395A -> 438A -0.12393
396A -> 438A -0.30473
397A -> 437A -0.35213
399A -> 437A 0.12108
411A -> 437A -0.10225
412A -> 437A -0.14071
413A -> 438A 0.11990
414A -> 438A 0.10585
415A -> 437A 0.16636
418A -> 438A 0.21641
419A -> 437A -0.20530
421A -> 438A 0.17927
395B -> 438B 0.12393
396B -> 438B 0.30473
397B -> 437B 0.35213
399B -> 437B -0.12107
411B -> 437B 0.10227
412B -> 437B 0.14073
413B -> 438B -0.11993
414B -> 438B -0.10586
415B -> 437B -0.16637
418B -> 438B -0.21642
419B -> 437B 0.20531
421B -> 438B -0.17927

Excited State 93: 3.000-A 2.4639 eV 503.21 nm f=0.0000 <S**2>=2.000

433A -> 439A -0.43091
434A -> 440A 0.53952
433B -> 439B 0.43080
434B -> 440B -0.53939

Excited State 94: 1.000-A 2.4658 eV 502.81 nm f=0.0002 <S**2>=0.000
433A -> 439A -0.44219
434A -> 440A 0.54231
433B -> 439B -0.44229
434B -> 440B 0.54245

Excited State 95: 3.000-A 2.4780 eV 500.34 nm f=0.0000 <S**2>=2.000
433A -> 440A 0.60590
434A -> 439A -0.29356
433B -> 440B -0.60586
434B -> 439B 0.29354

Excited State 96: 3.000-A 2.4801 eV 499.92 nm f=0.0000 <S**2>=2.000
407A -> 440A -0.47820
408A -> 439A -0.48963
407B -> 440B 0.47820
408B -> 439B 0.48963

Excited State 97: 3.000-A 2.4804 eV 499.86 nm f=0.0000 <S**2>=2.000
407A -> 439A -0.48939
408A -> 440A -0.46918
433A -> 440A -0.10462
407B -> 439B 0.48939
408B -> 440B 0.46918
433B -> 440B 0.10461

Excited State 98: 1.000-A 2.4816 eV 499.62 nm f=0.0002 <S**2>=0.000
433A -> 440A 0.62980
434A -> 439A -0.29057
433B -> 440B 0.62985
434B -> 439B -0.29059

Excited State 99: 1.000-A 2.5016 eV 495.61 nm f=0.0505 <S**2>=0.000

| | |
|---|---|
| 409A -> 438A | 0.12598 |
| 410A -> 437A | -0.15634 |
| 413A -> 437A | -0.17834 |
| 417A -> 437A | 0.50168 |
| 418A -> 437A | -0.33510 |
| 420A -> 438A | -0.12337 |
| 409B -> 438B | 0.12597 |
| 410B -> 437B | -0.15633 |
| 413B -> 437B | -0.17834 |
| 417B -> 437B | 0.50167 |
| 418B -> 437B | -0.33508 |
| 420B -> 438B | -0.12336 |

Excited State 100: 1.000-A 2.5167 eV 492.66 nm f=0.0022 <S**2>=0.000

| | |
|---|---|
| 409A -> 437A | -0.13330 |
| 410A -> 438A | 0.11214 |
| 411A -> 437A | -0.24035 |
| 412A -> 437A | -0.30288 |
| 413A -> 438A | 0.34987 |
| 414A -> 438A | 0.13684 |
| 416A -> 437A | 0.23967 |
| 419A -> 437A | -0.25014 |
| 421A -> 438A | 0.11273 |
| 409B -> 437B | -0.13330 |
| 410B -> 438B | 0.11214 |
| 411B -> 437B | -0.24035 |
| 412B -> 437B | -0.30287 |
| 413B -> 438B | 0.34987 |
| 414B -> 438B | 0.13683 |
| 416B -> 437B | 0.23968 |
| 419B -> 437B | -0.25013 |
| 421B -> 438B | 0.11272 |

Excited State 101: 1.000-A 2.5195 eV 492.10 nm f=0.0096 <S**2>=0.000

411A -> 438A -0.20772
412A -> 438A -0.24017
413A -> 437A 0.40627
414A -> 437A 0.16541
416A -> 438A 0.17233
417A -> 437A 0.29645
419A -> 438A -0.15100
411B -> 438B -0.20772
412B -> 438B -0.24016
413B -> 437B 0.40627
414B -> 437B 0.16539
416B -> 438B 0.17232
417B -> 437B 0.29644
419B -> 438B -0.15099

Excited State 102: 1.000-A 2.5278 eV 490.48 nm f=0.0022 <S**2>=0.000
409A -> 437A 0.17107
410A -> 438A -0.13471
416A -> 437A 0.42410
417A -> 438A 0.30400
418A -> 438A -0.32460
419A -> 437A -0.10555
409B -> 437B 0.17106
410B -> 438B -0.13470
416B -> 437B 0.42411
417B -> 438B 0.30397
418B -> 438B -0.32459
419B -> 437B -0.10556

Excited State 103: 3.000-A 2.5316 eV 489.75 nm f=0.0000 <S**2>=2.000
429A -> 442A -0.10900
431A -> 441A 0.15107
433A -> 442A -0.20902
434A -> 441A -0.23827
435A -> 442A -0.27931
436A -> 441A -0.47247

429B -> 442B 0.10901
431B -> 441B -0.15107
433B -> 442B 0.20902
434B -> 441B 0.23827
435B -> 442B 0.27931
436B -> 441B 0.47247

Excited State 104: 3.000-A 2.5442 eV 487.32 nm f=0.0000 <S**2>=2.000
429A -> 441A -0.12060
431A -> 442A 0.14003
433A -> 441A -0.24204
434A -> 442A -0.22080
435A -> 441A -0.36374
436A -> 442A -0.40096
429B -> 441B 0.12060
431B -> 442B -0.14003
433B -> 441B 0.24204
434B -> 442B 0.22080
435B -> 441B 0.36374
436B -> 442B 0.40096

Excited State 105: 3.000-A 2.5694 eV 482.54 nm f=0.0000 <S**2>=2.000
415A -> 437A -0.17129
416A -> 437A -0.49510
417A -> 438A 0.39978
419A -> 437A 0.14174
421A -> 438A -0.12148
415B -> 437B 0.17128
416B -> 437B 0.49519
417B -> 438B -0.39999
419B -> 437B -0.14177
421B -> 438B 0.12148

Excited State 106: 3.000-A 2.5722 eV 482.02 nm f=0.0000 <S**2>=2.000
416A -> 438A 0.27198
417A -> 437A -0.45022

418A -> 437A -0.17903
419A -> 438A -0.39186
416B -> 438B -0.27216
417B -> 437B 0.45046
418B -> 437B 0.17935
419B -> 438B 0.39233

Excited State 107: 1.000-A 2.5769 eV 481.14 nm f=0.0157 <S**2>=0.000
416A -> 438A -0.15931
417A -> 437A 0.26444
418A -> 437A 0.35369
419A -> 438A 0.50208
416B -> 438B -0.15904
417B -> 437B 0.26403
418B -> 437B 0.35353
419B -> 438B 0.50174

Excited State 108: 1.000-A 2.5819 eV 480.20 nm f=0.0091 <S**2>=0.000
411A -> 437A -0.12061
412A -> 437A -0.12016
415A -> 437A 0.12975
416A -> 437A -0.24138
417A -> 438A 0.56955
418A -> 438A 0.12426
419A -> 437A 0.20728
411B -> 437B -0.12057
412B -> 437B -0.12015
415B -> 437B 0.12983
416B -> 437B -0.24119
417B -> 438B 0.56946
418B -> 438B 0.12432
419B -> 437B 0.20728

Excited State 109: 3.000-A 2.5981 eV 477.21 nm f=0.0000 <S**2>=2.000
413A -> 438A 0.16023
415A -> 437A -0.16252

416A -> 437A -0.19410
417A -> 438A -0.28994
418A -> 438A -0.41278
419A -> 437A -0.33440
413B -> 438B -0.16069
415B -> 437B 0.16330
416B -> 437B 0.19519
417B -> 438B 0.28962
418B -> 438B 0.41423
419B -> 437B 0.33510

Excited State 110: 1.000-A 2.5992 eV 477.01 nm f=0.0023 <S**2>=0.000
413A -> 438A -0.14251
415A -> 437A 0.25124
416A -> 437A 0.33033
418A -> 438A 0.46059
419A -> 437A 0.23087
413B -> 438B -0.14200
415B -> 437B 0.25070
416B -> 437B 0.32966
418B -> 438B 0.45928
419B -> 437B 0.22983

Excited State 111: 3.000-A 2.6007 eV 476.74 nm f=0.0000 <S**2>=2.000
432A -> 439A -0.68854
432B -> 439B 0.68859

Excited State 112: 3.000-A 2.6032 eV 476.28 nm f=0.0000 <S**2>=2.000
413A -> 437A 0.15864
415A -> 438A -0.18019
416A -> 438A -0.51032
418A -> 437A -0.29353
419A -> 438A -0.23879
421A -> 437A -0.10636
413B -> 437B -0.15870
415B -> 438B 0.18026

416B -> 438B 0.51057
418B -> 437B 0.29358
419B -> 438B 0.23880
421B -> 437B 0.10639

Excited State 113: 1.000-A 2.6067 eV 475.64 nm f=0.0015 <S**2>=0.000
432A -> 439A 0.69590
432B -> 439B 0.69585

Excited State 114: 1.000-A 2.6149 eV 474.14 nm f=0.0041 <S**2>=0.000
409A -> 438A 0.10851
410A -> 437A -0.12967
413A -> 437A -0.13571
415A -> 438A 0.20689
416A -> 438A 0.58271
417A -> 437A -0.10100
418A -> 437A 0.18129
409B -> 438B 0.10850
410B -> 437B -0.12967
413B -> 437B -0.13565
415B -> 438B 0.20682
416B -> 438B 0.58250
417B -> 437B -0.10097
418B -> 437B 0.18118

Excited State 115: 3.000-A 2.6523 eV 467.46 nm f=0.0000 <S**2>=2.000
430A -> 439A 0.16274
432A -> 440A -0.67420
430B -> 439B -0.16275
432B -> 440B 0.67425

Excited State 116: 1.000-A 2.6589 eV 466.30 nm f=0.0000 <S**2>=0.000
430A -> 439A -0.12073
432A -> 440A 0.68647
430B -> 439B -0.12072
432B -> 440B 0.68643

Excited State 117: 3.000-A 2.6629 eV 465.60 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 404A -> 438A | -0.14839 |
| 406A -> 437A | -0.10888 |
| 409A -> 437A | 0.18153 |
| 411A -> 437A | -0.10239 |
| 413A -> 438A | 0.18148 |
| 414A -> 438A | -0.15045 |
| 415A -> 437A | -0.43545 |
| 416A -> 437A | 0.10863 |
| 417A -> 438A | -0.14121 |
| 418A -> 438A | 0.30165 |
| 419A -> 437A | 0.11423 |
| 404B -> 438B | 0.14840 |
| 406B -> 437B | 0.10887 |
| 409B -> 437B | -0.18150 |
| 411B -> 437B | 0.10241 |
| 413B -> 438B | -0.18150 |
| 414B -> 438B | 0.15051 |
| 415B -> 437B | 0.43563 |
| 416B -> 437B | -0.10868 |
| 417B -> 438B | 0.14114 |
| 418B -> 438B | -0.30173 |
| 419B -> 437B | -0.11426 |

Excited State 118: 3.000-A 2.6671 eV 464.87 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 404A -> 437A | -0.18457 |
| 406A -> 438A | -0.10430 |
| 409A -> 438A | 0.14345 |
| 413A -> 437A | 0.21530 |
| 414A -> 437A | -0.29154 |
| 415A -> 438A | -0.40144 |
| 417A -> 437A | -0.11403 |
| 418A -> 437A | 0.20442 |
| 419A -> 438A | 0.14083 |
| 404B -> 437B | 0.18458 |

406B -> 438B 0.10430
409B -> 438B -0.14344
413B -> 437B -0.21531
414B -> 437B 0.29160
415B -> 438B 0.40150
417B -> 437B 0.11402
418B -> 437B -0.20443
419B -> 438B -0.14084

Excited State 119: 1.000-A 2.6718 eV 464.05 nm f=0.0014 <S**2>=0.000
396A -> 438A -0.10182
397A -> 437A -0.10197
409A -> 437A 0.16618
410A -> 438A -0.15282
412A -> 437A -0.10913
414A -> 438A 0.13063
415A -> 437A 0.47214
416A -> 437A -0.16901
417A -> 438A -0.15743
418A -> 438A -0.20809
435A -> 443A -0.12549
436A -> 444A 0.12046
396B -> 438B -0.10183
397B -> 437B -0.10200
409B -> 437B 0.16624
410B -> 438B -0.15285
412B -> 437B -0.10911
414B -> 438B 0.13057
415B -> 437B 0.47199
416B -> 437B -0.16897
417B -> 438B -0.15747
418B -> 438B -0.20797
435B -> 443B -0.12548
436B -> 444B 0.12046

Excited State 120: 1.000-A 2.6834 eV 462.04 nm f=0.0299 <S**2>=0.000

396A -> 437A 0.12419
397A -> 438A 0.10203
409A -> 438A -0.19120
410A -> 437A 0.33771
414A -> 437A -0.27579
415A -> 438A -0.31716
416A -> 438A 0.18013
435A -> 444A -0.14188
436A -> 443A 0.15098
396B -> 437B 0.12419
397B -> 438B 0.10204
409B -> 438B -0.19122
410B -> 437B 0.33773
414B -> 437B -0.27575
415B -> 438B -0.31710
416B -> 438B 0.18012
435B -> 444B -0.14188
436B -> 443B 0.15099

Excited State 121: 3.000-A 2.6933 eV 460.34 nm f=0.0000 <S**2>=2.000
429A -> 440A 0.17003
430A -> 440A -0.27396
431A -> 439A -0.57373
433A -> 440A -0.15548
434A -> 439A -0.12005
429B -> 440B -0.17004
430B -> 440B 0.27396
431B -> 439B 0.57374
433B -> 440B 0.15548
434B -> 439B 0.12006

Excited State 122: 1.000-A 2.7032 eV 458.66 nm f=0.0051 <S**2>=0.000
431A -> 439A 0.18476
434A -> 441A 0.10840
435A -> 442A 0.24242
436A -> 441A 0.59694

431B -> 439B 0.18476
434B -> 441B 0.10840
435B -> 442B 0.24242
436B -> 441B 0.59694

Excited State 123: 3.000-A 2.7034 eV 458.63 nm f=0.0000 <S**2>=2.000
429A -> 439A 0.22476
430A -> 439A -0.36547
431A -> 440A -0.38266
433A -> 439A -0.12175
434A -> 440A -0.11608
435A -> 444A 0.19581
436A -> 443A -0.22962
429B -> 439B -0.22476
430B -> 439B 0.36547
431B -> 440B 0.38267
433B -> 439B 0.12175
434B -> 440B 0.11608
435B -> 444B -0.19581
436B -> 443B 0.22962

Excited State 124: 3.000-A 2.7076 eV 457.91 nm f=0.0000 <S**2>=2.000
429A -> 439A 0.12581
430A -> 439A -0.20390
431A -> 440A -0.20755
435A -> 444A -0.35696
436A -> 443A 0.42053
429B -> 439B -0.12582
430B -> 439B 0.20391
431B -> 440B 0.20756
435B -> 444B 0.35696
436B -> 443B -0.42053

Excited State 125: 3.000-A 2.7121 eV 457.15 nm f=0.0000 <S**2>=2.000
434A -> 444A 0.12606
435A -> 443A 0.48051

436A -> 444A -0.40435
434B -> 444B -0.12607
435B -> 443B -0.48051
436B -> 444B 0.40435

Excited State 126: 1.000-A 2.7126 eV 457.07 nm f=0.0001 <S**2>=0.000
429A -> 440A -0.16550
430A -> 440A 0.26244
431A -> 439A 0.57082
433A -> 440A 0.12445
434A -> 439A 0.10617
436A -> 441A -0.19184
429B -> 440B -0.16550
430B -> 440B 0.26244
431B -> 439B 0.57081
433B -> 440B 0.12444
434B -> 439B 0.10617
436B -> 441B -0.19184

Excited State 127: 1.000-A 2.7212 eV 455.61 nm f=0.0031 <S**2>=0.000
429A -> 439A -0.22379
430A -> 439A 0.38875
431A -> 440A 0.38033
433A -> 439A 0.10153
434A -> 440A 0.10013
435A -> 441A 0.25026
436A -> 442A 0.22803
429B -> 439B -0.22379
430B -> 439B 0.38874
431B -> 440B 0.38032
433B -> 439B 0.10153
434B -> 440B 0.10013
435B -> 441B 0.25026
436B -> 442B 0.22803

Excited State 128: 1.000-A 2.7279 eV 454.50 nm f=0.0080 <S**2>=0.000

410A -> 437A -0.18261
412A -> 438A 0.12166
413A -> 437A 0.19573
415A -> 438A -0.14566
429A -> 439A 0.11154
430A -> 439A -0.20366
431A -> 440A -0.20842
435A -> 441A 0.35414
436A -> 442A 0.33390
410B -> 437B -0.18261
412B -> 438B 0.12167
413B -> 437B 0.19572
415B -> 438B -0.14564
429B -> 439B 0.11154
430B -> 439B -0.20366
431B -> 440B -0.20842
435B -> 441B 0.35414
436B -> 442B 0.33390

Excited State 129: 1.000-A 2.7310 eV 453.99 nm f=0.0003 <S**2>=0.000
409A -> 438A 0.10627
410A -> 437A -0.25564
412A -> 438A 0.21660
413A -> 437A 0.32831
414A -> 437A -0.13254
415A -> 438A -0.30163
435A -> 441A -0.23449
436A -> 442A -0.21491
409B -> 438B 0.10625
410B -> 437B -0.25564
412B -> 438B 0.21662
413B -> 437B 0.32829
414B -> 437B -0.13254
415B -> 438B -0.30160
435B -> 441B -0.23449
436B -> 442B -0.21491

Excited State 130: 3.000-A 2.7352 eV 453.29 nm f=0.0000 <S**2>=2.000

406A -> 437A -0.17369
411A -> 437A 0.37882
412A -> 437A -0.50382
414A -> 438A 0.10578
415A -> 437A -0.13105
406B -> 437B 0.17369
411B -> 437B -0.37942
412B -> 437B 0.50460
414B -> 438B -0.10572
415B -> 437B 0.13075

Excited State 131: 1.000-A 2.7367 eV 453.05 nm f=0.0424 <S**2>=0.000

409A -> 437A 0.32052
410A -> 438A -0.26776
411A -> 437A -0.21415
412A -> 437A 0.29310
413A -> 438A 0.34604
415A -> 437A -0.17029
409B -> 437B 0.32044
410B -> 438B -0.26778
411B -> 437B -0.21327
412B -> 437B 0.29195
413B -> 438B 0.34582
415B -> 437B -0.17058

Excited State 132: 1.000-A 2.7545 eV 450.12 nm f=0.0112 <S**2>=0.000

406A -> 437A -0.17849
410A -> 438A -0.17258
411A -> 437A 0.39205
412A -> 437A -0.34982
414A -> 438A 0.22387
415A -> 437A -0.26671
406B -> 437B -0.17843
410B -> 438B -0.17261

411B -> 437B 0.39200
412B -> 437B -0.34966
414B -> 438B 0.22394
415B -> 437B -0.26665

Excited State 133: 3.000-A 2.7546 eV 450.09 nm f=0.0000 <S**2>=2.000
411A -> 438A -0.31558
414A -> 437A -0.50297
415A -> 438A 0.32525
411B -> 438B 0.31574
414B -> 437B 0.50326
415B -> 438B -0.32545

Excited State 134: 3.000-A 2.7628 eV 448.77 nm f=0.0000 <S**2>=2.000
409A -> 437A 0.12821
410A -> 438A 0.15029
411A -> 437A -0.32491
412A -> 437A -0.26134
413A -> 438A -0.29501
414A -> 438A -0.38648
415A -> 437A 0.12157
409B -> 437B -0.12829
410B -> 438B -0.15026
411B -> 437B 0.32494
412B -> 437B 0.26146
413B -> 438B 0.29505
414B -> 438B 0.38651
415B -> 437B -0.12149

Excited State 135: 1.000-A 2.7652 eV 448.38 nm f=0.0005 <S**2>=0.000
411A -> 438A 0.28504
414A -> 437A 0.53586
415A -> 438A -0.31078
411B -> 438B 0.28490
414B -> 437B 0.53563
415B -> 438B -0.31065

Excited State 136: 3.000-A 2.7721 eV 447.27 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 404A -> 437A | -0.14279 |
| 406A -> 438A | -0.19527 |
| 411A -> 438A | 0.11519 |
| 412A -> 438A | -0.58579 |
| 413A -> 437A | -0.21768 |
| 404B -> 437B | 0.14283 |
| 406B -> 438B | 0.19531 |
| 411B -> 438B | -0.11517 |
| 412B -> 438B | 0.58588 |
| 413B -> 437B | 0.21766 |

Excited State 137: 1.000-A 2.7787 eV 446.19 nm f=0.0240 <S**2>=0.000

| | |
|---|---|
| 406A -> 437A | 0.13964 |
| 409A -> 437A | -0.28789 |
| 411A -> 437A | 0.33384 |
| 412A -> 437A | 0.34055 |
| 413A -> 438A | 0.23040 |
| 414A -> 438A | 0.27446 |
| 415A -> 437A | 0.13737 |
| 406B -> 437B | 0.13961 |
| 409B -> 437B | -0.28786 |
| 411B -> 437B | 0.33378 |
| 412B -> 437B | 0.34047 |
| 413B -> 438B | 0.23035 |
| 414B -> 438B | 0.27435 |
| 415B -> 437B | 0.13739 |

Excited State 138: 1.000-A 2.8029 eV 442.34 nm f=0.0027 <S**2>=0.000

| | |
|---|---|
| 404A -> 437A | 0.16215 |
| 406A -> 438A | 0.20465 |
| 410A -> 437A | 0.13141 |
| 411A -> 438A | -0.15410 |
| 412A -> 438A | 0.55788 |
| 414A -> 437A | 0.13745 |

415A -> 438A 0.19257
404B -> 437B 0.16212
406B -> 438B 0.20464
410B -> 437B 0.13147
411B -> 438B -0.15422
412B -> 438B 0.55780
414B -> 437B 0.13752
415B -> 438B 0.19250

Excited State 139: 3.000-A 2.8083 eV 441.49 nm f=0.0000 <S**2>=2.000
409A -> 438A 0.28712
410A -> 437A 0.14588
411A -> 438A -0.45353
413A -> 437A -0.27597
414A -> 437A 0.24929
415A -> 438A -0.15422
409B -> 438B -0.28724
410B -> 437B -0.14584
411B -> 438B 0.45365
413B -> 437B 0.27605
414B -> 437B -0.24928
415B -> 438B 0.15435

Excited State 140: 3.000-A 2.8110 eV 441.07 nm f=0.0000 <S**2>=2.000
406A -> 437A -0.11727
409A -> 437A -0.22840
411A -> 437A 0.23304
413A -> 438A 0.30992
414A -> 438A -0.45297
415A -> 437A 0.19274
406B -> 437B 0.11735
409B -> 437B 0.22847
411B -> 437B -0.23312
413B -> 438B -0.31007
414B -> 438B 0.45327
415B -> 437B -0.19280

Excited State 141: 3.000-A 2.8210 eV 439.50 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 429A -> 439A | 0.16507 |
| 429A -> 441A | 0.18959 |
| 431A -> 442A | -0.17818 |
| 432A -> 442A | -0.10810 |
| 433A -> 441A | 0.15605 |
| 433A -> 448A | -0.12085 |
| 434A -> 447A | 0.10174 |
| 435A -> 448A | -0.12241 |
| 436A -> 442A | -0.26632 |
| 436A -> 445A | 0.17480 |
| 436A -> 447A | 0.15482 |
| 429B -> 439B | -0.16507 |
| 429B -> 441B | -0.18959 |
| 431B -> 442B | 0.17818 |
| 432B -> 442B | 0.10810 |
| 433B -> 441B | -0.15605 |
| 433B -> 448B | 0.12085 |
| 434B -> 447B | -0.10174 |
| 435B -> 448B | 0.12241 |
| 436B -> 442B | 0.26632 |
| 436B -> 445B | -0.17480 |
| 436B -> 447B | -0.15482 |

Excited State 142: 1.000-A 2.8211 eV 439.49 nm f=0.0081 <S**2>=0.000

| | |
|---|---|
| 406A -> 437A | 0.13604 |
| 409A -> 437A | 0.14668 |
| 410A -> 438A | 0.13633 |
| 411A -> 437A | -0.16787 |
| 413A -> 438A | -0.31094 |
| 414A -> 438A | 0.52201 |
| 415A -> 437A | -0.12068 |
| 406B -> 437B | 0.13597 |
| 409B -> 437B | 0.14656 |
| 410B -> 438B | 0.13628 |

411B -> 437B -0.16775
413B -> 438B -0.31076
414B -> 438B 0.52176
415B -> 437B -0.12057

Excited State 143: 1.000-A 2.8231 eV 439.18 nm f=0.0012 <S**2>=0.000
409A -> 438A -0.31308
411A -> 438A 0.50329
413A -> 437A 0.23867
414A -> 437A -0.13777
415A -> 438A 0.22782
409B -> 438B -0.31297
411B -> 438B 0.50312
413B -> 437B 0.23857
414B -> 437B -0.13769
415B -> 438B 0.22776

Excited State 144: 3.000-A 2.8317 eV 437.84 nm f=0.0000 <S**2>=2.000
429A -> 442A 0.18254
430A -> 440A 0.15187
431A -> 441A -0.20978
431A -> 448A 0.10447
432A -> 441A -0.11363
433A -> 447A 0.12115
434A -> 441A 0.17215
434A -> 448A -0.10579
435A -> 442A -0.22046
435A -> 445A 0.14471
435A -> 447A 0.13293
436A -> 441A -0.15828
436A -> 448A -0.14735
429B -> 442B -0.18254
430B -> 440B -0.15187
431B -> 441B 0.20978
431B -> 448B -0.10447
432B -> 441B 0.11363

433B -> 447B -0.12114
434B -> 441B -0.17215
434B -> 448B 0.10579
435B -> 442B 0.22047
435B -> 445B -0.14471
435B -> 447B -0.13293
436B -> 441B 0.15828
436B -> 448B 0.14735

Excited State 145: 3.000-A 2.8403 eV 436.52 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.31771
430A -> 439A -0.50949
431A -> 440A 0.31606
432A -> 440A -0.14451
429B -> 439B 0.31774
430B -> 439B 0.50953
431B -> 440B -0.31608
432B -> 440B 0.14452

Excited State 146: 1.000-A 2.8434 eV 436.04 nm f=0.0002 <S**2>=0.000
429A -> 439A 0.32136
430A -> 439A 0.51172
431A -> 440A -0.33493
432A -> 440A 0.13416
429B -> 439B 0.32134
430B -> 439B 0.51168
431B -> 440B -0.33490
432B -> 440B 0.13415

Excited State 147: 3.000-A 2.8537 eV 434.47 nm f=0.0000 <S**2>=2.000
431A -> 440A 0.11691
434A -> 442A 0.12020
435A -> 441A -0.53831
436A -> 442A 0.34432
431B -> 440B -0.11691
434B -> 442B -0.12020

435B -> 441B 0.53831
436B -> 442B -0.34433

Excited State 148: 1.000-A 2.8582 eV 433.78 nm f=0.0033 <S**2>=0.000
435A -> 441A -0.48050
436A -> 442A 0.49780
435B -> 441B -0.48029
436B -> 442B 0.49769

Excited State 149: 3.000-A 2.8583 eV 433.77 nm f=0.0000 <S**2>=2.000
402A -> 437A 0.18355
404A -> 437A 0.16239
406A -> 438A 0.14379
409A -> 438A -0.26582
410A -> 437A -0.44104
411A -> 438A -0.17207
412A -> 438A -0.11522
413A -> 437A -0.17390
415A -> 438A -0.16713
435A -> 441A -0.11837
402B -> 437B -0.18358
404B -> 437B -0.16242
406B -> 438B -0.14383
409B -> 438B 0.26594
410B -> 437B 0.44111
411B -> 438B 0.17208
412B -> 438B 0.11522
413B -> 437B 0.17394
415B -> 438B 0.16714
435B -> 441B 0.11914

Excited State 150: 3.000-A 2.8603 eV 433.46 nm f=0.0000 <S**2>=2.000
430A -> 440A -0.24777
431A -> 439A 0.13342
433A -> 442A -0.13478
435A -> 442A -0.43398

436A -> 441A 0.40174
430B -> 440B 0.24777
431B -> 439B -0.13342
433B -> 442B 0.13478
435B -> 442B 0.43398
436B -> 441B -0.40174

Excited State 151: 3.000-A 2.8670 eV 432.45 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.29498
410A -> 438A -0.44823
411A -> 437A -0.14582
413A -> 438A -0.15934
415A -> 437A -0.12249
430A -> 440A 0.23910
431A -> 439A -0.14001
435A -> 442A -0.11817
409B -> 437B 0.29509
410B -> 438B 0.44839
411B -> 437B 0.14587
413B -> 438B 0.15940
415B -> 437B 0.12252
430B -> 440B -0.23911
431B -> 439B 0.14002
435B -> 442B 0.11818

Excited State 152: 3.000-A 2.8695 eV 432.07 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.17077
410A -> 438A -0.22958
430A -> 440A -0.45395
431A -> 439A 0.26269
435A -> 442A 0.12542
436A -> 441A -0.20269
409B -> 437B 0.17085
410B -> 438B 0.22970
430B -> 440B 0.45395
431B -> 439B -0.26269

435B -> 442B -0.12541
436B -> 441B 0.20268

Excited State 153: 1.000-A 2.8700 eV 432.00 nm f=0.0005 <S**2>=0.000
430A -> 440A 0.62991
431A -> 439A -0.30491
430B -> 440B 0.62991
431B -> 439B -0.30491

Excited State 154: 1.000-A 2.8750 eV 431.25 nm f=0.0027 <S**2>=0.000
402A -> 437A -0.10338
404A -> 437A -0.11068
406A -> 438A -0.17216
409A -> 438A 0.44709
410A -> 437A 0.42195
411A -> 438A 0.16568
413A -> 437A 0.15790
402B -> 437B -0.10334
404B -> 437B -0.11064
406B -> 438B -0.17212
409B -> 438B 0.44703
410B -> 437B 0.42184
411B -> 438B 0.16564
413B -> 437B 0.15786

Excited State 155: 1.000-A 2.8767 eV 431.00 nm f=0.0000 <S**2>=0.000
409A -> 437A 0.36814
410A -> 438A 0.51208
411A -> 437A 0.17489
413A -> 438A 0.18295
409B -> 437B 0.36802
410B -> 438B 0.51190
411B -> 437B 0.17483
413B -> 438B 0.18289

Excited State 156: 3.000-A 2.8804 eV 430.44 nm f=0.0000 <S**2>=2.000

391A -> 439A 0.11699
429A -> 439A -0.47898
430A -> 439A 0.10383
431A -> 440A -0.38327
435A -> 441A -0.11309
391B -> 439B -0.11698
429B -> 439B 0.48968
430B -> 439B -0.10574
431B -> 440B 0.39113
435B -> 441B 0.11319

Excited State 157: 1.000-A 2.8804 eV 430.44 nm f=0.0004 <S**2>=0.000
429A -> 439A 0.55954
431A -> 440A 0.41063
429B -> 439B 0.55018
431B -> 440B 0.40317

Excited State 158: 1.000-A 2.8847 eV 429.80 nm f=0.0005 <S**2>=0.000
433A -> 442A 0.11705
435A -> 442A 0.62564
436A -> 441A -0.27413
433B -> 442B 0.11705
435B -> 442B 0.62564
436B -> 441B -0.27412

Excited State 159: 3.000-A 2.9028 eV 427.12 nm f=0.0000 <S**2>=2.000
390A -> 439A 0.28893
391A -> 440A 0.31514
401A -> 439A 0.10608
429A -> 440A -0.39357
430A -> 440A -0.22530
390B -> 439B -0.28893
391B -> 440B -0.31514
401B -> 439B -0.10608
429B -> 440B 0.39360
430B -> 440B 0.22531

Excited State 160: 3.000-A 2.9089 eV 426.22 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 394A -> 438A | -0.11834 |
| 396A -> 437A | 0.12082 |
| 401A -> 437A | 0.10275 |
| 402A -> 437A | -0.34079 |
| 404A -> 437A | -0.16441 |
| 405A -> 437A | 0.31172 |
| 406A -> 438A | -0.12237 |
| 409A -> 438A | -0.34937 |
| 411A -> 438A | -0.13642 |
| 394B -> 438B | 0.11835 |
| 396B -> 437B | -0.12080 |
| 401B -> 437B | -0.10278 |
| 402B -> 437B | 0.34086 |
| 404B -> 437B | 0.16443 |
| 405B -> 437B | -0.31180 |
| 406B -> 438B | 0.12241 |
| 409B -> 438B | 0.34941 |
| 411B -> 438B | 0.13644 |

Excited State 161: 3.000-A 2.9096 eV 426.13 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 390A -> 440A | -0.36152 |
| 391A -> 439A | -0.41167 |
| 392A -> 440A | -0.11541 |
| 400A -> 439A | -0.12743 |
| 401A -> 440A | -0.11398 |
| 429A -> 439A | -0.18343 |
| 390B -> 440B | 0.36152 |
| 391B -> 439B | 0.41167 |
| 392B -> 440B | 0.11541 |
| 400B -> 439B | 0.12743 |
| 401B -> 440B | 0.11398 |
| 429B -> 439B | 0.18342 |

Excited State 162: 3.000-A 2.9125 eV 425.69 nm f=0.0000 <S**2>=2.000

394A -> 437A -0.13090
396A -> 438A 0.10314
400A -> 437A 0.12093
402A -> 438A -0.30073
404A -> 438A -0.13366
405A -> 438A 0.26613
406A -> 437A -0.33621
409A -> 437A -0.26862
411A -> 437A -0.12992
414A -> 438A 0.10521
394B -> 437B 0.13091
396B -> 438B -0.10313
400B -> 437B -0.12096
402B -> 438B 0.30078
404B -> 438B 0.13367
405B -> 438B -0.26618
406B -> 437B 0.33629
409B -> 437B 0.26865
411B -> 437B 0.12994
414B -> 438B -0.10522

Excited State 163: 1.000-A 2.9187 eV 424.79 nm f=0.0001 <S**2>=0.000
429A -> 440A 0.67006
430A -> 440A 0.10592
431A -> 439A 0.15211
429B -> 440B 0.67014
430B -> 440B 0.10591
431B -> 439B 0.15213

Excited State 164: 3.000-A 2.9239 eV 424.04 nm f=0.0000 <S**2>=2.000
390A -> 439A 0.24254
391A -> 440A 0.26059
429A -> 440A 0.53597
431A -> 439A 0.12015
390B -> 439B -0.24254
391B -> 440B -0.26059

429B -> 440B -0.53585
431B -> 439B -0.12012

Excited State 165: 1.000-A 2.9299 eV 423.17 nm f=0.0049 <S**2>=0.000
396A -> 437A -0.23175
397A -> 438A -0.24384
401A -> 437A 0.19459
402A -> 437A -0.24313
405A -> 437A 0.36258
406A -> 438A -0.16900
409A -> 438A -0.11893
435A -> 444A -0.11674
436A -> 443A 0.20138
396B -> 437B -0.23176
397B -> 438B -0.24383
401B -> 437B 0.19461
402B -> 437B -0.24307
405B -> 437B 0.36256
406B -> 438B -0.16900
409B -> 438B -0.11886
435B -> 444B -0.11674
436B -> 443B 0.20139

Excited State 166: 1.000-A 2.9404 eV 421.66 nm f=0.0515 <S**2>=0.000
396A -> 438A 0.15402
397A -> 437A 0.24482
401A -> 438A -0.13769
402A -> 438A 0.21080
405A -> 438A -0.27359
406A -> 437A 0.39444
409A -> 437A 0.16367
412A -> 437A -0.10365
435A -> 443A -0.13273
436A -> 444A 0.11342
396B -> 438B 0.15404
397B -> 437B 0.24482

401B -> 438B -0.13769
402B -> 438B 0.21074
405B -> 438B -0.27355
406B -> 437B 0.39440
409B -> 437B 0.16363
412B -> 437B -0.10364
435B -> 443B -0.13273
436B -> 444B 0.11343

Excited State 167: 1.000-A 2.9566 eV 419.35 nm f=0.0011 <S**2>=0.000
396A -> 437A -0.21629
397A -> 438A -0.12282
402A -> 437A 0.30163
404A -> 437A 0.28480
405A -> 437A -0.19360
406A -> 438A 0.14339
409A -> 438A 0.19382
411A -> 438A 0.12812
435A -> 444A -0.14833
436A -> 443A 0.27197
396B -> 437B -0.21621
397B -> 438B -0.12271
402B -> 437B 0.30185
404B -> 437B 0.28623
405B -> 437B -0.19270
406B -> 438B 0.14253
409B -> 438B 0.19415
411B -> 438B 0.12831
435B -> 444B -0.14835
436B -> 443B 0.27202

Excited State 168: 3.000-A 2.9570 eV 419.29 nm f=0.0000 <S**2>=2.000
401A -> 437A 0.23010
404A -> 437A 0.44978
405A -> 437A 0.26761
406A -> 438A -0.26294

409A -> 438A 0.10917
414A -> 437A -0.11181
415A -> 438A -0.13968
401B -> 437B -0.23013
404B -> 437B -0.44891
405B -> 437B -0.26822
406B -> 438B 0.26341
409B -> 438B -0.10857
414B -> 437B 0.11168
415B -> 438B 0.13964

Excited State 169: 1.000-A 2.9658 eV 418.04 nm f=0.0845 <S**2>=0.000
396A -> 438A -0.25927
397A -> 437A -0.28841
399A -> 437A 0.13942
400A -> 437A -0.10796
406A -> 437A 0.31977
411A -> 437A 0.10234
414A -> 438A -0.10508
435A -> 443A 0.26090
436A -> 444A -0.23875
396B -> 438B -0.25925
397B -> 437B -0.28841
399B -> 437B 0.13942
400B -> 437B -0.10795
406B -> 437B 0.31976
411B -> 437B 0.10234
414B -> 438B -0.10508
435B -> 443B 0.26090
436B -> 444B -0.23875

Excited State 170: 3.000-A 2.9746 eV 416.81 nm f=0.0000 <S**2>=2.000
394A -> 437A -0.12389
401A -> 438A -0.14602
402A -> 438A -0.21734
403A -> 437A 0.10601

404A -> 438A -0.44666
406A -> 437A 0.32842
435A -> 442A 0.11123
394B -> 437B 0.12390
401B -> 438B 0.14603
402B -> 438B 0.21739
403B -> 437B -0.10601
404B -> 438B 0.44672
406B -> 437B -0.32840
435B -> 442B -0.11123

Excited State 171: 1.000-A 2.9907 eV 414.57 nm f=0.0048 <S**2>=0.000
396A -> 437A 0.14297
397A -> 438A 0.13806
401A -> 437A 0.16921
402A -> 437A 0.17333
404A -> 437A 0.45587
405A -> 437A 0.16880
406A -> 438A -0.21598
435A -> 444A 0.11767
436A -> 443A -0.22995
396B -> 437B 0.14298
397B -> 438B 0.13808
401B -> 437B 0.16922
402B -> 437B 0.17332
404B -> 437B 0.45586
405B -> 437B 0.16883
406B -> 438B -0.21598
435B -> 444B 0.11779
436B -> 443B -0.22993

Excited State 172: 3.000-A 2.9911 eV 414.51 nm f=0.0000 <S**2>=2.000
429A -> 441A 0.13891
431A -> 442A -0.13959
433A -> 441A 0.17388
433A -> 448A 0.11339

434A -> 442A 0.15850
434A -> 443A -0.15096
435A -> 441A -0.10553
435A -> 444A -0.11088
435A -> 448A 0.12367
436A -> 442A -0.32445
436A -> 445A -0.16353
436A -> 447A -0.15943
429B -> 441B -0.13891
431B -> 442B 0.13959
433B -> 441B -0.17389
433B -> 448B -0.11340
434B -> 442B -0.15850
434B -> 443B 0.15099
435B -> 441B 0.10553
435B -> 444B 0.11076
435B -> 448B -0.12368
436B -> 442B 0.32448
436B -> 445B 0.16355
436B -> 447B 0.15945

Excited State 173: 3.000-A 2.9969 eV 413.70 nm f=0.0000 <S**2>=2.000
404A -> 438A -0.15182
406A -> 437A 0.11540
431A -> 441A -0.12165
431A -> 448A -0.11506
433A -> 442A 0.11085
433A -> 443A -0.11062
433A -> 445A -0.11196
433A -> 447A -0.11550
434A -> 441A 0.18801
434A -> 448A 0.10987
435A -> 442A -0.32394
435A -> 445A -0.14053
435A -> 447A -0.14606
436A -> 448A 0.15945

404B -> 438B 0.15185
406B -> 437B -0.11541
431B -> 441B 0.12165
431B -> 448B 0.11506
433B -> 442B -0.11085
433B -> 443B 0.11062
433B -> 445B 0.11196
433B -> 447B 0.11550
434B -> 441B -0.18801
434B -> 448B -0.10987
435B -> 442B 0.32394
435B -> 445B 0.14053
435B -> 447B 0.14606
436B -> 448B -0.15945

Excited State 174: 1.000-A 3.0231 eV 410.12 nm f=0.0007 <S**2>=0.000
401A -> 438A 0.11631
402A -> 438A 0.34537
404A -> 438A 0.53815
406A -> 437A -0.17887
401B -> 438B 0.11629
402B -> 438B 0.34534
404B -> 438B 0.53809
406B -> 437B -0.17884

Excited State 175: 3.000-A 3.0291 eV 409.32 nm f=0.0000 <S**2>=2.000
427A -> 440A 0.16061
428A -> 439A 0.67164
427B -> 440B -0.16061
428B -> 439B -0.67163

Excited State 176: 3.000-A 3.0309 eV 409.07 nm f=0.0000 <S**2>=2.000
401A -> 438A -0.22805
402A -> 438A 0.18399
404A -> 438A -0.15865
405A -> 438A -0.39187

406A -> 437A -0.29485
409A -> 437A -0.11167
412A -> 437A 0.12572
414A -> 438A 0.19713
401B -> 438B 0.22811
402B -> 438B -0.18404
404B -> 438B 0.15869
405B -> 438B 0.39198
406B -> 437B 0.29490
409B -> 437B 0.11169
412B -> 437B -0.12574
414B -> 438B -0.19717

Excited State 177: 3.000-A 3.0341 eV 408.64 nm f=0.0000 <S**2>=2.000
400A -> 438A 0.12646
401A -> 437A -0.11526
402A -> 437A 0.14881
403A -> 438A -0.11769
405A -> 437A -0.25752
406A -> 438A -0.48750
409A -> 438A -0.16515
411A -> 438A -0.11526
412A -> 438A 0.16569
414A -> 437A 0.13855
400B -> 438B -0.12652
401B -> 437B 0.11532
402B -> 437B -0.14888
403B -> 438B 0.11775
405B -> 437B 0.25766
406B -> 438B 0.48777
409B -> 438B 0.16523
411B -> 438B 0.11533
412B -> 438B -0.16577
414B -> 437B -0.13862

Excited State 178: 1.000-A 3.0343 eV 408.61 nm f=0.0001 <S**2>=0.000

407A -> 440A 0.23714
408A -> 439A 0.25073
427A -> 440A 0.13117
428A -> 439A 0.59119
407B -> 440B 0.23714
408B -> 439B 0.25073
427B -> 440B 0.13118
428B -> 439B 0.59121

Excited State 179: 1.000-A 3.0439 eV 407.33 nm f=0.0052 <S**2>=0.000
400A -> 438A -0.12492
401A -> 437A 0.10548
402A -> 437A -0.13840
403A -> 438A 0.11686
405A -> 437A 0.24237
406A -> 438A 0.50883
409A -> 438A 0.14159
411A -> 438A 0.13253
412A -> 438A -0.13701
414A -> 437A -0.13156
436A -> 443A -0.14125
400B -> 438B -0.12486
401B -> 437B 0.10542
402B -> 437B -0.13832
403B -> 438B 0.11679
405B -> 437B 0.24223
406B -> 438B 0.50857
409B -> 438B 0.14150
411B -> 438B 0.13247
412B -> 438B -0.13692
414B -> 437B -0.13149
436B -> 443B -0.14124

Excited State 180: 1.000-A 3.0447 eV 407.21 nm f=0.0000 <S**2>=0.000
407A -> 439A 0.49298
408A -> 440A 0.46961

428A -> 440A 0.10455
407B -> 439B 0.49298
408B -> 440B 0.46961
428B -> 440B 0.10455

Excited State 181: 1.000-A 3.0487 eV 406.67 nm f=0.0000 <S**2>=0.000
407A -> 440A 0.41422
408A -> 439A 0.43316
428A -> 439A -0.34721
407B -> 440B 0.41422
408B -> 439B 0.43316
428B -> 439B -0.34721

Excited State 182: 1.000-A 3.0494 eV 406.58 nm f=0.0013 <S**2>=0.000
401A -> 438A 0.22473
402A -> 438A -0.20511
404A -> 438A 0.14687
405A -> 438A 0.42841
406A -> 437A 0.24885
414A -> 438A -0.17516
435A -> 443A -0.15478
436A -> 444A 0.13867
401B -> 438B 0.22467
402B -> 438B -0.20506
404B -> 438B 0.14683
405B -> 438B 0.42831
406B -> 437B 0.24877
414B -> 438B -0.17511
435B -> 443B -0.15478
436B -> 444B 0.13867

Excited State 183: 3.000-A 3.0666 eV 404.30 nm f=0.0000 <S**2>=2.000
405A -> 437A -0.10402
431A -> 443A -0.10090
433A -> 441A -0.10354
433A -> 444A 0.24264

434A -> 443A -0.30439
435A -> 444A -0.12705
435A -> 450A -0.17742
436A -> 443A -0.18858
436A -> 449A -0.22801
405B -> 437B 0.10402
431B -> 443B 0.10090
433B -> 441B 0.10354
433B -> 444B -0.24264
434B -> 443B 0.30439
435B -> 444B 0.12705
435B -> 450B 0.17742
436B -> 443B 0.18859
436B -> 449B 0.22801

Excited State 184: 3.000-A 3.0724 eV 403.54 nm f=0.0000 <S**2>=2.000
427A -> 439A 0.31177
428A -> 440A 0.61127
427B -> 439B -0.31177
428B -> 440B -0.61127

Excited State 185: 3.000-A 3.0810 eV 402.42 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.10772
405A -> 438A -0.14353
408A -> 437A 0.23646
430A -> 443A -0.12141
433A -> 443A -0.25469
434A -> 444A 0.24504
435A -> 449A -0.25847
436A -> 450A -0.21759
393B -> 437B -0.10773
405B -> 438B 0.14351
408B -> 437B -0.23673
430B -> 443B 0.12141
433B -> 443B 0.25469
434B -> 444B -0.24505

435B -> 449B 0.25848
436B -> 450B 0.21759

Excited State 186: 1.000-A 3.0849 eV 401.90 nm f=0.0005 <S**2>=0.000
427A -> 439A 0.27970
428A -> 440A 0.62869
427B -> 439B 0.27970
428B -> 440B 0.62867

Excited State 187: 1.000-A 3.0856 eV 401.82 nm f=0.0001 <S**2>=0.000
408A -> 437A 0.68283
408B -> 437B 0.68989

Excited State 188: 3.000-A 3.0860 eV 401.76 nm f=0.0000 <S**2>=2.000
408A -> 437A 0.65232
408B -> 437B -0.64473

Excited State 189: 1.000-A 3.1080 eV 398.92 nm f=0.0140 <S**2>=0.000
396A -> 437A -0.12245
407A -> 437A 0.59929
408A -> 438A 0.21531
436A -> 443A -0.18917
396B -> 437B -0.12238
407B -> 437B 0.60173
408B -> 438B 0.21615
436B -> 443B -0.18912

Excited State 190: 3.000-A 3.1093 eV 398.76 nm f=0.0000 <S**2>=2.000
407A -> 437A 0.65696
408A -> 438A 0.22751
407B -> 437B -0.65484
408B -> 438B -0.22673

Excited State 191: 1.000-A 3.1149 eV 398.04 nm f=0.0561 <S**2>=0.000
396A -> 437A 0.27225
397A -> 438A 0.19848

405A -> 437A 0.24632
407A -> 437A 0.26829
436A -> 443A 0.36742
396B -> 437B 0.27224
397B -> 438B 0.19848
405B -> 437B 0.24628
407B -> 437B 0.26801
436B -> 443B 0.36742

Excited State 192: 3.000-A 3.1259 eV 396.63 nm f=0.0000 <S**2>=2.000
392A -> 437A 0.10588
393A -> 438A 0.13517
433A -> 450A 0.11281
434A -> 449A 0.14822
435A -> 444A 0.27479
435A -> 450A -0.24470
436A -> 443A 0.35484
436A -> 449A -0.20869
392B -> 437B -0.10589
393B -> 438B -0.13518
433B -> 450B -0.11281
434B -> 449B -0.14822
435B -> 444B -0.27478
435B -> 450B 0.24470
436B -> 443B -0.35483
436B -> 449B 0.20869

Excited State 193: 3.000-A 3.1374 eV 395.18 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.13417
433A -> 443A -0.16321
434A -> 444A 0.15372
435A -> 443A 0.28967
435A -> 449A 0.11914
436A -> 444A 0.48230
393B -> 437B 0.13417
433B -> 443B 0.16321

434B -> 444B -0.15372
435B -> 443B -0.28965
435B -> 449B -0.11913
436B -> 444B -0.48228

Excited State 194: 3.000-A 3.1433 eV 394.44 nm f=0.0000 <S**2>=2.000
402A -> 437A 0.32907
403A -> 438A 0.19926
404A -> 437A -0.17448
405A -> 437A 0.28751
407A -> 437A 0.13242
408A -> 438A -0.44003
402B -> 437B -0.33008
403B -> 438B -0.19986
404B -> 437B 0.17503
405B -> 437B -0.28830
407B -> 437B -0.13291
408B -> 438B 0.44164

Excited State 195: 1.000-A 3.1447 eV 394.26 nm f=0.0018 <S**2>=0.000
402A -> 437A -0.29377
403A -> 438A -0.17867
404A -> 437A 0.16128
405A -> 437A -0.23395
407A -> 437A -0.15164
408A -> 438A 0.49270
402B -> 437B -0.29267
403B -> 438B -0.17800
404B -> 437B 0.16069
405B -> 437B -0.23299
407B -> 437B -0.15121
408B -> 438B 0.49125

Excited State 196: 3.000-A 3.1487 eV 393.76 nm f=0.0000 <S**2>=2.000
402A -> 438A -0.19041
403A -> 437A -0.61971

405A -> 438A -0.16287
406A -> 437A 0.15133
402B -> 438B 0.19208
403B -> 437B 0.62540
405B -> 438B 0.16450
406B -> 437B -0.15263

Excited State 197: 1.000-A 3.1493 eV 393.69 nm f=0.0011 <S**2>=0.000
402A -> 438A 0.18471
403A -> 437A 0.62596
405A -> 438A 0.17955
406A -> 437A -0.14261
402B -> 438B 0.18297
403B -> 437B 0.62030
405B -> 438B 0.17805
406B -> 437B -0.14122

Excited State 198: 3.000-A 3.1523 eV 393.31 nm f=0.0000 <S**2>=2.000
402A -> 437A -0.31174
403A -> 438A -0.12150
404A -> 437A 0.18289
405A -> 437A -0.24884
407A -> 437A 0.17828
408A -> 438A -0.48247
402B -> 437B 0.31315
403B -> 438B 0.12208
404B -> 437B -0.18364
405B -> 437B 0.24983
407B -> 437B -0.17896
408B -> 438B 0.48421

Excited State 199: 1.000-A 3.1535 eV 393.16 nm f=0.0012 <S**2>=0.000
402A -> 437A 0.35698
403A -> 438A 0.14650
404A -> 437A -0.18887
405A -> 437A 0.25182

| | |
|---|---|
| 407A -> 437A | -0.17290 |
| 408A -> 438A | 0.44254 |
| 402B -> 437B | 0.35572 |
| 403B -> 438B | 0.14601 |
| 404B -> 437B | -0.18813 |
| 405B -> 437B | 0.25082 |
| 407B -> 437B | -0.17221 |
| 408B -> 438B | 0.44069 |

Excited State 200: 1.000-A 3.1551 eV 392.96 nm f=0.0248 <S**2>=0.000

| | |
|---|---|
| 397A -> 437A | 0.15500 |
| 435A -> 443A | 0.53341 |
| 436A -> 444A | 0.30094 |
| 397B -> 437B | 0.15500 |
| 435B -> 443B | 0.53343 |
| 436B -> 444B | 0.30097 |

**Table S10.** Standard orientation of the optimized geometry for the open-ring isomer (OF3) of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | -0.18024 | -2.14154 | -0.21421 |
| N | -4.46048 | -2.55754 | 0.14895 |
| C | -3.41173 | -1.94397 | -0.51338 |
| C | -3.9597 | -1.22071 | -1.65747 |
| C | -5.36079 | -1.44221 | -1.66196 |
| C | -5.79125 | -2.34473 | -0.47736 |
| C | -6.74106 | -1.60105 | 0.436099 |
| C | -8.02737 | -1.95941 | 0.589833 |
| C | -8.588 | -3.16357 | -0.05481 |
| C | -7.65047 | -3.9928 | -0.83741 |
| C | -6.36323 | -3.64517 | -1.00486 |
| O | -9.79383 | -3.47519 | 0.072178 |
| C | -3.3761 | -0.46763 | -2.68178 |
| C | -4.20336 | 0.058606 | -3.68426 |
| C | -5.58839 | -0.1589 | -3.67762 |
| C | -6.17903 | -0.91927 | -2.65482 |
| C | -3.96517 | -3.40561 | 1.136753 |
| C | -2.58365 | -3.27231 | 1.05803 |
| N | -2.25309 | -2.34826 | 0.035624 |
| C | -4.83165 | -4.2572 | 1.979145 |
| C | -1.46792 | -3.96515 | 1.676591 |
| C | -1.59301 | -4.89171 | 2.72688 |
| C | -0.48035 | -5.61383 | 3.159835 |
| C | 0.753347 | -5.42082 | 2.52689 |
| C | 0.885903 | -4.47753 | 1.500448 |
| C | -0.20379 | -3.69481 | 1.075824 |
| C | -5.65377 | -3.69254 | 2.972049 |
| C | -6.48546 | -4.50437 | 3.74991 |
| C | -6.50106 | -5.8897 | 3.551965 |
| C | -5.67882 | -6.46251 | 2.573772 |
| C | -4.85159 | -5.65319 | 1.790518 |
| N | -4.00137 | 2.946959 | -0.16512 |
| C | -3.02761 | 2.216077 | 0.491191 |
| C | -3.65346 | 1.545001 | 1.627767 |
| C | -5.02099 | 1.92041 | 1.634309 |
| C | -5.34998 | 2.87072 | 0.455139 |
| C | -5.78684 | 4.220852 | 0.98633 |
| C | -7.03007 | 4.700543 | 0.813554 |
| C | -8.04385 | 3.976381 | 0.021098 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -7.60692 | 2.724084 | -0.62709 | C | 0.224741 | -4.32827 | -4.50899 |
| C | -6.3655 | 2.233793 | -0.46841 | C | -1.03565 | -4.31261 | -3.89988 |
| O | -9.2098 | 4.41254 | -0.11029 | C | -1.19816 | -3.76552 | -2.62028 |
| C | -3.15858 | 0.71644 | 2.639935 | C | -0.11165 | -3.22122 | -1.91484 |
| C | -4.03974 | 0.274479 | 3.636962 | C | 5.651825 | -2.90308 | -3.20874 |
| C | -5.39077 | 0.648528 | 3.635821 | C | 6.540142 | -3.52179 | -4.094 |
| C | -5.89273 | 1.481418 | 2.622198 | C | 6.364552 | -4.8647 | -4.44635 |
| C | -3.4189 | 3.737601 | -1.15262 | C | 5.293774 | -5.58899 | -3.90773 |
| C | -2.06144 | 3.450498 | -1.07863 | C | 4.410166 | -4.97731 | -3.01495 |
| N | -1.83325 | 2.494998 | -0.05882 | N | 4.563354 | 1.764254 | 0.840705 |
| C | -4.18596 | 4.679142 | -1.99541 | C | 3.514047 | 1.671762 | -0.07168 |
| C | -0.87801 | 3.993222 | -1.71747 | C | 3.834066 | 1.430083 | -1.45388 |
| C | -0.8969 | 4.912293 | -2.78148 | C | 2.938454 | 0.777933 | -2.33135 |
| C | 0.297138 | 5.452446 | -3.25996 | C | 3.340139 | 0.362647 | -3.58919 |
| C | 1.51028 | 5.080454 | -2.66728 | C | 4.665149 | 0.586588 | -4.02625 |
| C | 1.530739 | 4.148548 | -1.62348 | C | 5.554088 | 1.264065 | -3.21046 |
| C | 0.350098 | 3.5598 | -1.14205 | C | 4.051867 | 2.234765 | 1.990602 |
| C | -5.06547 | 4.207908 | -2.98796 | C | 2.62114 | 2.383985 | 1.822468 |
| C | -5.80018 | 5.106876 | -3.76753 | N | 2.299158 | 1.953665 | 0.541675 |
| C | -5.66044 | 6.485595 | -3.57183 | C | 4.940065 | 2.517135 | 3.131332 |
| C | -4.7797 | 6.964553 | -2.59418 | C | 1.561981 | 2.951025 | 2.597745 |
| C | -4.04893 | 6.06877 | -1.80906 | C | 1.666899 | 3.391853 | 3.940089 |
| Cl | -0.23367 | 0.150683 | -1.64771 | C | 0.616779 | 4.078696 | 4.530635 |
| Cl | -0.07315 | -0.1901 | 1.645214 | C | -0.54994 | 4.349404 | 3.786322 |
| Ir | 0.199534 | 2.054527 | 0.196971 | C | -0.69014 | 3.872563 | 2.484024 |
| N | 4.078316 | -2.50568 | -0.44468 | C | 0.329979 | 3.114322 | 1.87092 |
| C | 2.980302 | -2.11671 | 0.300106 | C | 5.936577 | 1.584482 | 3.479209 |
| C | 3.402731 | -1.93055 | 1.685458 | C | 6.840813 | 1.85919 | 4.507153 |
| C | 4.78661 | -2.22455 | 1.741956 | C | 6.778288 | 3.076663 | 5.196405 |
| C | 5.350333 | -2.54587 | 0.335962 | C | 5.808487 | 4.021714 | 4.842845 |
| C | 5.972867 | -3.92338 | 0.300919 | C | 4.898194 | 3.747094 | 3.818223 |
| C | 7.285289 | -4.12063 | 0.090191 | H | -6.32787 | -0.72929 | 0.93335 |
| C | 8.20734 | -3.00445 | -0.20033 | H | -8.70756 | -1.39037 | 1.214485 |
| C | 7.616381 | -1.65444 | -0.26242 | H | -8.05436 | -4.90717 | -1.25803 |
| C | 6.305202 | -1.43542 | -0.05818 | H | -5.67434 | -4.26187 | -1.57455 |
| O | 9.430346 | -3.19758 | -0.39113 | H | -2.31052 | -0.28741 | -2.69191 |
| C | 2.70784 | -1.64486 | 2.865197 | H | -3.75358 | 0.636971 | -4.48439 |
| C | 3.412547 | -1.64436 | 4.075935 | H | -6.20676 | 0.246793 | -4.47154 |
| C | 4.783746 | -1.92858 | 4.121661 | H | -7.24755 | -1.10958 | -2.65113 |
| C | 5.485258 | -2.2202 | 2.941743 | H | -2.55518 | -5.05445 | 3.198656 |
| C | 3.65767 | -3.00433 | -1.68133 | H | -0.57763 | -6.32823 | 3.971163 |
| C | 2.271775 | -2.86508 | -1.66809 | H | 1.618504 | -6.00041 | 2.837295 |
| N | 1.873537 | -2.28671 | -0.44094 | H | 1.854959 | -4.35273 | 1.035008 |
| C | 4.57849 | -3.6249 | -2.65358 | H | -5.62912 | -2.62051 | 3.136676 |
| C | 1.178637 | -3.30738 | -2.52212 | H | -7.11608 | -4.05732 | 4.511643 |
| C | 1.331228 | -3.82991 | -3.81791 | H | -7.14651 | -6.51842 | 4.156668 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -5.68466 | -7.5365 | 2.418609 | H | 5.78326 | -1.85876 | -2.95161 |
| H | -4.21151 | -6.09579 | 1.034374 | H | 7.366804 | -2.95471 | -4.50987 |
| H | -5.04183 | 4.760274 | 1.563791 | H | 7.055113 | -5.34258 | -5.13369 |
| H | -7.3401 | 5.649577 | 1.237064 | H | 5.151919 | -6.6312 | -4.17521 |
| H | -8.33753 | 2.231135 | -1.25935 | H | 3.585361 | -5.54124 | -2.5922 |
| H | -6.04194 | 1.326758 | -0.96868 | H | 1.940913 | 0.548621 | -1.99269 |
| H | -2.12089 | 0.41288 | 2.641667 | H | 2.635756 | -0.16383 | -4.22376 |
| H | -3.65939 | -0.36483 | 4.426532 | H | 4.976736 | 0.255418 | -5.01143 |
| H | -6.0507 | 0.305942 | 4.42607 | H | 6.542883 | 1.507743 | -3.58245 |
| H | -6.93337 | 1.789856 | 2.621707 | H | 2.563457 | 3.184048 | 4.509141 |
| H | -1.83771 | 5.206048 | -3.23204 | H | 0.695513 | 4.412941 | 5.559853 |
| H | 0.281526 | 6.161074 | -4.08182 | H | -1.35545 | 4.919681 | 4.240621 |
| H | 2.442667 | 5.510233 | -3.02232 | H | -1.60785 | 4.071426 | 1.944856 |
| H | 2.479838 | 3.864618 | -1.1928 | H | 5.989097 | 0.648363 | 2.93727 |
| H | -5.16083 | 3.139772 | -3.15173 | H | 7.598289 | 1.126365 | 4.767162 |
| H | -6.47611 | 4.732127 | -4.52931 | H | 7.485435 | 3.291727 | 5.991085 |
| H | -6.23081 | 7.181602 | -4.17825 | H | 5.770052 | 4.97922 | 5.352376 |
| H | -4.66495 | 8.032671 | -2.44107 | H | 4.174606 | 4.500509 | 3.527689 |
| H | -3.36415 | 6.438371 | -1.05276 | C | 5.153828 | 1.772708 | -1.941 |
| H | 5.297214 | -4.75038 | 0.498014 | C | 6.033238 | 2.71129 | -1.27677 |
| H | 7.722793 | -5.11289 | 0.103665 | C | 7.462491 | 2.5441 | -1.35873 |
| H | 8.299915 | -0.84143 | -0.48308 | C | 5.543588 | 3.921068 | -0.66283 |
| H | 5.879058 | -0.43625 | -0.0792 | C | 8.323215 | 3.454189 | -0.81532 |
| H | 1.652437 | -1.41957 | 2.838757 | H | 7.851339 | 1.638741 | -1.81348 |
| H | 2.879501 | -1.42341 | 4.994401 | C | 6.3899 | 4.863791 | -0.15656 |
| H | 5.30645 | -1.92764 | 5.072184 | H | 4.475463 | 4.09831 | -0.65162 |
| H | 6.544715 | -2.45365 | 2.968327 | H | 9.397056 | 3.302986 | -0.82841 |
| H | 2.30956 | -3.8518 | -4.28458 | H | 6.018846 | 5.789849 | 0.267493 |
| H | 0.346769 | -4.73134 | -5.50944 | C | 7.836991 | 4.681008 | -0.18006 |
| H | -1.89649 | -4.71788 | -4.42495 | O | 8.637209 | 5.538298 | 0.299855 |
| H | -2.18709 | -3.75203 | -2.17728 | | | | |

Excited State 1: 3.000-A -0.5891 eV -2104.57 nm f=-0.0000 <S**2>=2.000

429A -> 437A 0.12566

430A -> 437A -0.11140

433A -> 438A 0.39984

435A -> 437A -0.54700

429B -> 437B -0.12566

430B -> 437B 0.11142

433B -> 438B -0.39984

435B -> 437B 0.54701

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -6023.98797584

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.000-A -0.5815 eV -2132.01 nm f=-0.0000 <S**2>=2.000

429A -> 438A -0.10717

433A -> 437A -0.45367

435A -> 438A 0.50403

429B -> 438B 0.10717

433B -> 437B 0.45369

435B -> 438B -0.50402

Excited State 3: 3.000-A 0.3157 eV 3927.44 nm f=0.0000 <S**2>=2.000

436A -> 437A -0.70286

436B -> 437B 0.70580

Excited State 4: 1.000-A 0.3249 eV 3815.79 nm f=0.0010 <S**2>=0.000

436A -> 437A 0.70646

436B -> 437B 0.70352

Excited State 5: 3.000-A 0.3955 eV 3134.99 nm f=0.0000 <S**2>=2.000

436A -> 438A -0.70116

436B -> 438B 0.70171

Excited State 6: 1.000-A 0.4202 eV 2950.82 nm f=0.0043 <S**2>=0.000

436A -> 438A 0.70615

436B -> 438B 0.70561

Excited State 7: 3.000-A 0.6551 eV 1892.47 nm f=0.0000 <S**2>=2.000

429A -> 438A -0.21583

430A -> 438A 0.18560

433A -> 437A -0.42270

435A -> 438A -0.48220

429B -> 438B 0.21584

430B -> 438B -0.18563

433B -> 437B 0.42277

435B -> 438B 0.48230

Excited State 8: 3.000-A 0.7401 eV 1675.28 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 429A -> 437A | -0.19669 |
| 430A -> 437A | 0.18236 |
| 433A -> 438A | -0.47267 |
| 435A -> 437A | -0.45010 |
| 429B -> 437B | 0.19673 |
| 430B -> 437B | -0.18242 |
| 433B -> 438B | 0.47276 |
| 435B -> 437B | 0.45034 |

Excited State 9: 1.000-A 0.7966 eV 1556.34 nm f=0.1334 <S**2>=0.000

| | |
|---|---|
| 433A -> 438A | 0.25630 |
| 435A -> 437A | 0.65180 |
| 433B -> 438B | 0.25612 |
| 435B -> 437B | 0.65164 |
| 435A <- 437A | -0.13669 |
| 435B <- 437B | -0.13668 |

Excited State 10: 1.000-A 0.7971 eV 1555.46 nm f=0.0019 <S**2>=0.000

| | |
|---|---|
| 433A -> 437A | 0.40046 |
| 435A -> 438A | 0.56681 |
| 433B -> 437B | 0.40038 |
| 435B -> 438B | 0.56674 |

Excited State 11: 3.000-A 0.8437 eV 1469.50 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 432A -> 437A | -0.10725 |
| 434A -> 437A | -0.68792 |
| 432B -> 437B | 0.10771 |
| 434B -> 437B | 0.69126 |

Excited State 12: 1.000-A 0.8518 eV 1455.61 nm f=0.0009 <S**2>=0.000

| | |
|---|---|
| 434A -> 437A | 0.69243 |
| 435A -> 438A | -0.10286 |
| 434B -> 437B | 0.68908 |
| 435B -> 438B | -0.10291 |

Excited State 13: 3.000-A 0.9135 eV 1357.20 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 428A -> 438A | 0.13553 |
| 432A -> 438A | -0.16622 |
| 434A -> 438A | -0.66103 |
| 428B -> 438B | -0.13564 |
| 432B -> 438B | 0.16644 |
| 434B -> 438B | 0.66208 |

Excited State 14: 1.000-A 0.9287 eV 1334.97 nm f=0.0045 <S**2>=0.000

| | |
|---|---|
| 432A -> 438A | 0.12746 |
| 434A -> 438A | 0.68345 |
| 432B -> 438B | 0.12721 |
| 434B -> 438B | 0.68242 |

Excited State 15: 3.000-A 1.0408 eV 1191.28 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 428A -> 437A | 0.25423 |
| 430A -> 438A | -0.10633 |
| 432A -> 437A | -0.59195 |
| 433A -> 437A | -0.18934 |
| 434A -> 437A | 0.13283 |
| 428B -> 437B | -0.25457 |
| 430B -> 438B | 0.10640 |
| 432B -> 437B | 0.59337 |
| 433B -> 437B | 0.18988 |
| 434B -> 437B | -0.13305 |

Excited State 16: 1.000-A 1.0578 eV 1172.11 nm f=0.0018 <S**2>=0.000

| | |
|---|---|
| 428A -> 437A | -0.13447 |
| 432A -> 437A | 0.62204 |
| 433A -> 437A | 0.24213 |
| 435A -> 438A | -0.15055 |
| 428B -> 437B | -0.13388 |
| 432B -> 437B | 0.62070 |
| 433B -> 437B | 0.24168 |
| 435B -> 438B | -0.15056 |

Excited State 17: 3.000-A 1.0727 eV 1155.82 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 428A -> 438A | 0.40113 |
| 429A -> 437A | 0.11837 |
| 430A -> 437A | -0.17274 |
| 431A -> 437A | 0.13283 |
| 432A -> 438A | -0.42499 |
| 433A -> 438A | -0.17935 |
| 434A -> 438A | 0.22185 |
| 428B -> 438B | -0.40150 |
| 429B -> 437B | -0.11849 |
| 430B -> 437B | 0.17299 |
| 431B -> 437B | -0.13302 |
| 432B -> 438B | 0.42554 |
| 433B -> 438B | 0.17999 |
| 434B -> 438B | -0.22206 |

Excited State 18: 1.000-A 1.0946 eV 1132.64 nm f=0.0461 <S**2>=0.000

| | |
|---|---|
| 428A -> 438A | -0.21479 |
| 430A -> 437A | 0.16659 |
| 431A -> 437A | -0.13630 |
| 432A -> 438A | 0.39508 |
| 433A -> 438A | 0.45779 |
| 434A -> 438A | -0.13317 |
| 435A -> 437A | -0.14618 |
| 428B -> 438B | -0.21420 |
| 430B -> 437B | 0.16641 |
| 431B -> 437B | -0.13610 |
| 432B -> 438B | 0.39441 |
| 433B -> 438B | 0.45756 |
| 434B -> 438B | -0.13289 |
| 435B -> 437B | -0.14615 |

Excited State 19: 3.000-A 1.1565 eV 1072.06 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 423A -> 438A | -0.13021 |
| 424A -> 437A | -0.14776 |

428A -> 438A -0.13344
429A -> 437A 0.22556
430A -> 437A -0.50421
431A -> 437A -0.21708
432A -> 438A 0.17540
433A -> 438A -0.22762
423B -> 438B 0.13019
424B -> 437B 0.14774
428B -> 438B 0.13364
429B -> 437B -0.22581
430B -> 437B 0.50511
431B -> 437B 0.21772
432B -> 438B -0.17611
433B -> 438B 0.22801

Excited State 20: 3.000-A 1.1705 eV 1059.26 nm f=0.0000 <S**2>=2.000
423A -> 437A 0.36721
424A -> 438A 0.30317
429A -> 438A -0.24070
430A -> 438A 0.35668
432A -> 437A -0.15817
433A -> 437A 0.18076
423B -> 437B -0.36717
424B -> 438B -0.30311
429B -> 438B 0.24073
430B -> 438B -0.35681
432B -> 437B 0.15821
433B -> 437B -0.18087

Excited State 21: 3.000-A 1.1749 eV 1055.23 nm f=0.0000 <S**2>=2.000
423A -> 438A 0.40412
424A -> 437A 0.51447
425A -> 438A 0.11774
430A -> 437A -0.15487
423B -> 438B -0.40407
424B -> 437B -0.51441

425B -> 438B -0.11767
430B -> 437B 0.15922

Excited State 22: 1.000-A 1.1761 eV 1054.16 nm f=0.0130 <S**2>=0.000
429A -> 437A -0.13393
430A -> 437A 0.44566
431A -> 437A 0.32565
432A -> 438A -0.34603
433A -> 438A 0.23551
429B -> 437B -0.13300
430B -> 437B 0.44311
431B -> 437B 0.32460
432B -> 438B -0.34525
433B -> 438B 0.23447

Excited State 23: 3.000-A 1.1763 eV 1054.03 nm f=0.0000 <S**2>=2.000
423A -> 437A 0.36529
424A -> 438A 0.31656
425A -> 437A 0.12132
429A -> 438A 0.22082
430A -> 438A -0.34310
432A -> 437A 0.16762
433A -> 437A -0.16662
423B -> 437B -0.36526
424B -> 438B -0.31651
425B -> 437B -0.12123
429B -> 438B -0.22086
430B -> 438B 0.34323
432B -> 437B -0.16764
433B -> 437B 0.16670

Excited State 24: 3.000-A 1.2042 eV 1029.56 nm f=0.0000 <S**2>=2.000
426A -> 438A -0.11085
428A -> 437A -0.61981
430A -> 438A -0.13013
432A -> 437A -0.24591

426B -> 438B 0.11090
428B -> 437B 0.62028
430B -> 438B 0.13019
432B -> 437B 0.24612

Excited State 25: 3.000-A 1.2207 eV 1015.68 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.39847
430A -> 437A 0.10898
431A -> 437A -0.52368
432A -> 438A 0.16914
428B -> 438B -0.39882
430B -> 437B -0.10935
431B -> 437B 0.52474
432B -> 438B -0.16865

Excited State 26: 1.000-A 1.2351 eV 1003.80 nm f=0.0037 <S**2>=0.000
429A -> 437A 0.12818
431A -> 437A 0.58723
432A -> 438A 0.32337
433A -> 438A -0.10578
434A -> 438A -0.10808
429B -> 437B 0.12843
431B -> 437B 0.58717
432B -> 438B 0.32476
433B -> 438B -0.10563
434B -> 438B -0.10812

Excited State 27: 1.000-A 1.2450 eV 995.89 nm f=0.0085 <S**2>=0.000
428A -> 437A -0.34078
430A -> 438A 0.22018
432A -> 437A -0.30456
433A -> 437A 0.40666
435A -> 438A -0.30480
428B -> 437B -0.34035
430B -> 438B 0.22014
432B -> 437B -0.30435

433B -> 437B 0.40662
435B -> 438B -0.30482
433A <- 437A -0.11002
435A <- 438A 0.13975
433B <- 437B -0.11001
435B <- 438B 0.13975

Excited State 28: 3.000-A 1.2450 eV 995.83 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.31919
429A -> 437A 0.15481
431A -> 437A 0.37498
432A -> 438A 0.46412
428B -> 438B -0.31958
429B -> 437B -0.15458
431B -> 437B -0.37352
432B -> 438B -0.46355

Excited State 29: 1.000-A 1.2682 eV 977.61 nm f=0.0420 <S**2>=0.000
428A -> 438A 0.34800
429A -> 437A 0.19961
430A -> 437A 0.43402
431A -> 437A -0.14245
432A -> 438A 0.27223
433A -> 438A -0.19560
435A -> 437A 0.13995
428B -> 438B 0.34756
429B -> 437B 0.19993
430B -> 437B 0.43412
431B -> 437B -0.14250
432B -> 438B 0.27192
433B -> 438B -0.19571
435B -> 437B 0.13994

Excited State 30: 1.000-A 1.2758 eV 971.80 nm f=0.0001 <S**2>=0.000
428A -> 437A 0.36916
430A -> 438A 0.52904

431A -> 438A 0.25615
428B -> 437B 0.36888
430B -> 438B 0.52892
431B -> 438B 0.25621

Excited State 31: 3.000-A 1.3060 eV 949.35 nm f=0.0000 <S**2>=2.000
429A -> 437A -0.58167
430A -> 437A -0.35664
433A -> 438A 0.10336
429B -> 437B 0.58223
430B -> 437B 0.35662
433B -> 438B -0.10335

Excited State 32: 3.000-A 1.3103 eV 946.23 nm f=0.0000 <S**2>=2.000
429A -> 438A -0.20812
431A -> 438A -0.65731
429B -> 438B 0.20869
431B -> 438B 0.65996

Excited State 33: 1.000-A 1.3144 eV 943.28 nm f=0.0014 <S**2>=0.000
428A -> 437A -0.31032
429A -> 438A 0.12017
431A -> 438A 0.60549
433A -> 437A -0.10298
428B -> 437B -0.30991
429B -> 438B 0.11924
431B -> 438B 0.60255
433B -> 437B -0.10276

Excited State 34: 1.000-A 1.3314 eV 931.21 nm f=0.0031 <S**2>=0.000
428A -> 438A -0.45642
429A -> 437A 0.46926
430A -> 437A 0.18560
432A -> 438A -0.14253
428B -> 438B -0.45618
429B -> 437B 0.46847

430B -> 437B 0.18514
432B -> 438B -0.14243

Excited State 35: 3.000-A 1.3687 eV 905.84 nm f=0.0000 <S**2>=2.000
429A -> 438A -0.51957
430A -> 438A -0.41748
431A -> 438A 0.19520
429B -> 438B 0.52005
430B -> 438B 0.41782
431B -> 438B -0.19549

Excited State 36: 1.000-A 1.3858 eV 894.69 nm f=0.0015 <S**2>=0.000
428A -> 437A -0.28778
429A -> 438A 0.35007
430A -> 438A 0.36774
431A -> 438A -0.23945
433A -> 437A -0.26986
435A -> 438A 0.18980
428B -> 437B -0.28766
429B -> 438B 0.34948
430B -> 438B 0.36726
431B -> 438B -0.23925
433B -> 437B -0.26979
435B -> 438B 0.18984

Excited State 37: 1.000-A 1.4964 eV 828.54 nm f=0.0090 <S**2>=0.000
423A -> 437A -0.16979
424A -> 438A -0.13640
428A -> 437A 0.20080
429A -> 438A 0.57180
430A -> 438A -0.14689
433A -> 437A 0.17746
435A -> 438A -0.18086
423B -> 437B -0.16984
424B -> 438B -0.13643
428B -> 437B 0.20078

429B -> 438B 0.57170
430B -> 438B -0.14693
433B -> 437B 0.17748
435B -> 438B -0.18086

Excited State 38: 1.000-A 1.5012 eV 825.92 nm f=0.1472 <S**2>=0.000
423A -> 438A -0.18753
424A -> 437A -0.22090
428A -> 438A 0.30705
429A -> 437A 0.39826
430A -> 437A -0.16920
433A -> 438A 0.30645
435A -> 437A -0.21669
423B -> 438B -0.18756
424B -> 437B -0.22095
428B -> 438B 0.30703
429B -> 437B 0.39820
430B -> 437B -0.16922
433B -> 438B 0.30646
435B -> 437B -0.21669
433A <- 438A -0.10540
435A <- 437A 0.12267
433B <- 438B -0.10541
435B <- 437B 0.12268

Excited State 39: 1.000-A 1.5617 eV 793.91 nm f=0.0022 <S**2>=0.000
423A -> 437A 0.50063
424A -> 438A 0.41142
425A -> 437A 0.14138
429A -> 438A 0.16352
423B -> 437B 0.50076
424B -> 438B 0.41149
425B -> 437B 0.14131
429B -> 438B 0.16351

Excited State 40: 1.000-A 1.5649 eV 792.29 nm f=0.0416 <S**2>=0.000

423A -> 438A 0.37454
424A -> 437A 0.50272
425A -> 438A 0.12853
428A -> 438A 0.11314
429A -> 437A 0.17209
433A -> 438A 0.14745
435A -> 437A -0.10937
423B -> 438B 0.37462
424B -> 437B 0.50283
425B -> 438B 0.12848
428B -> 438B 0.11314
429B -> 437B 0.17207
433B -> 438B 0.14745
435B -> 437B -0.10937

Excited State 41: 3.000-A 1.6108 eV 769.68 nm f=0.0000 <S**2>=2.000
426A -> 438A -0.67291
428A -> 437A 0.12157
426B -> 438B 0.67334
428B -> 437B -0.12157

Excited State 42: 3.000-A 1.6410 eV 755.54 nm f=0.0000 <S**2>=2.000
426A -> 437A -0.67740
428A -> 438A 0.11959
426B -> 437B 0.67823
428B -> 438B -0.11957

Excited State 43: 1.000-A 1.6845 eV 736.04 nm f=0.0047 <S**2>=0.000
426A -> 437A 0.69861
426B -> 437B 0.69781

Excited State 44: 1.000-A 1.6928 eV 732.42 nm f=0.0002 <S**2>=0.000
426A -> 438A 0.69441
426B -> 438B 0.69399

Excited State 45: 3.000-A 1.7436 eV 711.08 nm f=0.0000 <S**2>=2.000

427A -> 437A -0.69516
427B -> 437B 0.69959

Excited State 46: 1.000-A 1.7496 eV 708.64 nm f=0.0001 <S**2>=0.000
427A -> 437A 0.70550
427B -> 437B 0.70110

Excited State 47: 3.000-A 1.8285 eV 678.06 nm f=0.0000 <S**2>=2.000
427A -> 438A -0.68683
427B -> 438B 0.68796

Excited State 48: 1.000-A 1.8401 eV 673.80 nm f=0.0004 <S**2>=0.000
427A -> 438A 0.70218
427B -> 438B 0.70107

Excited State 49: 3.000-A 1.8876 eV 656.85 nm f=0.0000 <S**2>=2.000
398A -> 438A -0.14400
399A -> 437A 0.18309
401A -> 438A 0.10640
405A -> 437A -0.11975
413A -> 437A -0.13107
419A -> 437A -0.13527
420A -> 438A 0.17777
421A -> 437A -0.36768
422A -> 438A -0.10057
425A -> 438A 0.33795
426A -> 437A 0.12000
398B -> 438B 0.14400
399B -> 437B -0.18309
401B -> 438B -0.10639
405B -> 437B 0.11974
413B -> 437B 0.13107
419B -> 437B 0.13528
420B -> 438B -0.17778
421B -> 437B 0.36774
422B -> 438B 0.10057

425B -> 438B -0.33803
426B -> 437B -0.11996

Excited State 50: 3.000-A 1.8878 eV 656.76 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.14424
399A -> 438A -0.14294
401A -> 437A -0.11230
413A -> 438A 0.10475
419A -> 438A 0.11542
420A -> 437A -0.19129
421A -> 438A 0.27967
422A -> 437A 0.11598
423A -> 437A 0.11555
425A -> 437A -0.44523
398B -> 437B -0.14424
399B -> 438B 0.14294
401B -> 437B 0.11229
413B -> 438B -0.10475
419B -> 438B -0.11543
420B -> 437B 0.19130
421B -> 438B -0.27971
422B -> 437B -0.11599
423B -> 437B -0.11551
425B -> 437B 0.44544

Excited State 51: 3.000-A 1.9744 eV 627.95 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.12955
399A -> 438A 0.12070
401A -> 437A 0.15686
405A -> 438A -0.12722
409A -> 437A 0.10450
411A -> 438A -0.11326
412A -> 437A -0.14987
413A -> 438A -0.13226
416A -> 437A 0.18240
420A -> 437A 0.20582

421A -> 438A -0.10978
423A -> 437A 0.12277
425A -> 437A -0.45798
398B -> 437B 0.12956
399B -> 438B -0.12070
401B -> 437B -0.15685
405B -> 438B 0.12720
409B -> 437B -0.10451
411B -> 438B 0.11327
412B -> 437B 0.14987
413B -> 438B 0.13225
416B -> 437B -0.18242
420B -> 437B -0.20584
421B -> 438B 0.10970
423B -> 437B -0.12288
425B -> 437B 0.45873

Excited State 52: 3.000-A 1.9954 eV 621.35 nm f=0.0000 <S**2>=2.000
399A -> 437A 0.10975
401A -> 438A 0.10282
405A -> 437A -0.12025
411A -> 437A -0.11184
413A -> 437A -0.12569
416A -> 438A 0.14709
420A -> 438A 0.14601
421A -> 437A -0.10375
423A -> 438A 0.13981
425A -> 438A -0.53425
427A -> 438A -0.12669
399B -> 437B -0.10976
401B -> 438B -0.10281
405B -> 437B 0.12023
411B -> 437B 0.11183
413B -> 437B 0.12569
416B -> 438B -0.14710
420B -> 438B -0.14602

421B -> 437B 0.10375
423B -> 438B -0.13976
425B -> 438B 0.53450
427B -> 438B 0.12670

Excited State 53: 1.000-A 2.0072 eV 617.70 nm f=0.0016 <S**2>=0.000
423A -> 437A -0.17384
425A -> 437A 0.67370
423B -> 437B -0.17356
425B -> 437B 0.67316

Excited State 54: 3.000-A 2.0153 eV 615.20 nm f=0.0000 <S**2>=2.000
436A -> 439A -0.69814
436B -> 439B 0.69816

Excited State 55: 1.000-A 2.0229 eV 612.91 nm f=0.0000 <S**2>=0.000
436A -> 439A 0.70026
436B -> 439B 0.70025

Excited State 56: 3.000-A 2.0291 eV 611.04 nm f=0.0000 <S**2>=2.000
436A -> 440A -0.69805
436B -> 440B 0.69807

Excited State 57: 1.000-A 2.0339 eV 609.58 nm f=0.0002 <S**2>=0.000
436A -> 440A 0.70000
436B -> 440B 0.69997

Excited State 58: 3.000-A 2.0629 eV 601.03 nm f=0.0000 <S**2>=2.000
401A -> 437A -0.11511
403A -> 437A -0.12428
405A -> 438A 0.11174
409A -> 437A -0.10000
411A -> 438A 0.16547
412A -> 437A 0.20932
413A -> 438A 0.16642
416A -> 437A -0.14158

420A -> 437A 0.12287
421A -> 438A -0.26922
422A -> 437A -0.36681
425A -> 437A -0.19477
401B -> 437B 0.11512
403B -> 437B 0.12429
405B -> 438B -0.11174
409B -> 437B 0.10001
411B -> 438B -0.16548
412B -> 437B -0.20936
413B -> 438B -0.16642
416B -> 437B 0.14159
420B -> 437B -0.12294
421B -> 438B 0.26936
422B -> 437B 0.36707
425B -> 437B 0.19463

Excited State 59: 3.000-A 2.0641 eV 600.66 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.12799
401A -> 438A -0.13451
403A -> 438A -0.10420
405A -> 437A 0.15983
409A -> 438A -0.10463
411A -> 437A 0.20575
412A -> 438A 0.19864
413A -> 437A 0.25027
416A -> 438A -0.12505
421A -> 437A -0.33233
422A -> 438A -0.18523
425A -> 438A -0.18774
400B -> 437B -0.12799
401B -> 438B 0.13453
403B -> 438B 0.10418
405B -> 437B -0.15982
409B -> 438B 0.10463
411B -> 437B -0.20577

412B -> 438B -0.19867
413B -> 437B -0.25033
416B -> 438B 0.12504
421B -> 437B 0.33253
422B -> 438B 0.18534
425B -> 438B 0.18815

Excited State 60: 1.000-A 2.0746 eV 597.63 nm f=0.0416 <S**2>=0.000
421A -> 437A -0.21640
423A -> 438A -0.15659
425A -> 438A 0.63924
421B -> 437B -0.21658
423B -> 438B -0.15640
425B -> 438B 0.63897

Excited State 61: 1.000-A 2.1214 eV 584.45 nm f=0.0335 <S**2>=0.000
420A -> 438A -0.15714
421A -> 437A 0.61345
422A -> 438A 0.17355
425A -> 438A 0.20270
420B -> 438B -0.15698
421B -> 437B 0.61348
422B -> 438B 0.17356
425B -> 438B 0.20258

Excited State 62: 3.000-A 2.1256 eV 583.29 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.14888
399A -> 438A -0.11989
400A -> 438A -0.20296
403A -> 437A 0.23800
416A -> 437A 0.19891
418A -> 438A 0.15066
420A -> 437A -0.14605
422A -> 437A -0.47960
398B -> 437B -0.14908
399B -> 438B 0.11993

400B -> 438B 0.20294
403B -> 437B -0.23785
416B -> 437B -0.19936
418B -> 438B -0.15062
420B -> 437B 0.14533
422B -> 437B 0.48524

Excited State 63: 1.000-A 2.1292 eV 582.31 nm f=0.0002 <S**2>=0.000
421A -> 438A 0.21140
422A -> 437A 0.65753
421B -> 438B 0.21125
422B -> 437B 0.65331

Excited State 64: 3.000-A 2.1458 eV 577.79 nm f=0.0000 <S**2>=2.000
398A -> 438A -0.17814
399A -> 437A 0.21046
400A -> 437A 0.27805
403A -> 438A -0.24599
416A -> 438A -0.19306
418A -> 437A -0.25453
419A -> 437A 0.10746
420A -> 438A 0.10505
421A -> 437A 0.21734
422A -> 438A 0.28451
398B -> 438B 0.17814
399B -> 437B -0.21046
400B -> 437B -0.27807
403B -> 438B 0.24601
416B -> 438B 0.19304
418B -> 437B 0.25463
419B -> 437B -0.10742
420B -> 438B -0.10521
421B -> 437B -0.21683
422B -> 438B -0.28447

Excited State 65: 3.000-A 2.1795 eV 568.85 nm f=0.0000 <S**2>=2.000

398A -> 437A 0.14278
399A -> 438A -0.13400
400A -> 438A -0.14632
403A -> 437A 0.18611
412A -> 437A 0.11044
416A -> 437A 0.18555
417A -> 437A 0.12421
418A -> 438A 0.13969
419A -> 438A -0.10740
421A -> 438A -0.42360
422A -> 437A 0.31330
398B -> 437B -0.14282
399B -> 438B 0.13402
400B -> 438B 0.14631
403B -> 437B -0.18612
412B -> 437B -0.11047
416B -> 437B -0.18573
417B -> 437B -0.12440
418B -> 438B -0.13965
419B -> 438B 0.10754
421B -> 438B 0.42460
422B -> 437B -0.31357

Excited State 66: 3.000-A 2.1839 eV 567.72 nm f=0.0000 <S**2>=2.000
418A -> 437A -0.10061
421A -> 437A 0.29539
422A -> 438A -0.58517
418B -> 437B 0.10065
421B -> 437B -0.29537
422B -> 438B 0.58571

Excited State 67: 1.000-A 2.1954 eV 564.74 nm f=0.0019 <S**2>=0.000
420A -> 437A -0.30829
421A -> 438A 0.55758
422A -> 437A -0.23599
420B -> 437B -0.30831

421B -> 438B 0.55684
422B -> 437B -0.23540

Excited State 68: 1.000-A 2.2209 eV 558.25 nm f=0.0066 <S**2>=0.000
421A -> 437A -0.15221
422A -> 438A 0.66321
421B -> 437B -0.15202
422B -> 438B 0.66274

Excited State 69: 1.000-A 2.2605 eV 548.49 nm f=0.0035 <S**2>=0.000
416A -> 438A 0.24382
418A -> 437A 0.51746
419A -> 437A -0.18634
420A -> 438A -0.30202
416B -> 438B 0.24461
418B -> 437B 0.51934
419B -> 437B -0.18722
420B -> 438B -0.30316

Excited State 70: 1.000-A 2.2605 eV 548.47 nm f=0.0004 <S**2>=0.000
416A -> 437A -0.34516
418A -> 438A -0.36087
419A -> 438A 0.14196
420A -> 437A 0.39143
421A -> 438A 0.18427
416B -> 437B -0.34605
418B -> 438B -0.36203
419B -> 438B 0.14243
420B -> 437B 0.39294
421B -> 438B 0.18419

Excited State 71: 3.000-A 2.2661 eV 547.13 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.15049
396A -> 438A -0.14417
399A -> 437A 0.13641
400A -> 437A 0.22386

403A -> 438A -0.20191
416A -> 438A 0.18932
418A -> 437A 0.41508
419A -> 437A -0.19885
420A -> 438A -0.25041
395B -> 437B 0.15043
396B -> 438B 0.14410
399B -> 437B -0.13656
400B -> 437B -0.22409
403B -> 438B 0.20211
416B -> 438B -0.18815
418B -> 437B -0.41264
419B -> 437B 0.19798
420B -> 438B 0.24896

Excited State 72: 3.000-A 2.2667 eV 546.98 nm f=0.0000 <S**2>=2.000
395A -> 438A 0.12934
396A -> 437A 0.18074
399A -> 438A -0.11812
400A -> 438A -0.18492
403A -> 437A 0.24596
416A -> 437A -0.23735
418A -> 438A -0.30342
419A -> 438A 0.12411
420A -> 437A 0.37108
395B -> 438B -0.12925
396B -> 437B -0.18067
399B -> 438B 0.11825
400B -> 438B 0.18509
403B -> 437B -0.24615
416B -> 437B 0.23591
418B -> 438B 0.30189
419B -> 438B -0.12353
420B -> 437B -0.36942

Excited State 73: 3.000-A 2.2852 eV 542.56 nm f=0.0000 <S**2>=2.000

398A -> 438A 0.16482
399A -> 437A -0.22493
400A -> 437A 0.18402
401A -> 438A -0.20467
403A -> 438A -0.11977
405A -> 437A 0.18694
410A -> 437A -0.10437
412A -> 438A -0.11369
413A -> 437A -0.33593
416A -> 438A 0.18020
418A -> 437A -0.11126
419A -> 437A -0.15994
420A -> 438A 0.18598
398B -> 438B -0.16484
399B -> 437B 0.22496
400B -> 437B -0.18403
401B -> 438B 0.20468
403B -> 438B 0.11975
405B -> 437B -0.18695
410B -> 437B 0.10440
412B -> 438B 0.11371
413B -> 437B 0.33608
416B -> 438B -0.18031
418B -> 437B 0.11122
419B -> 437B 0.16009
420B -> 438B -0.18600

Excited State 74: 3.000-A 2.2866 eV 542.22 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.21501
399A -> 438A -0.19894
400A -> 438A 0.17013
401A -> 437A -0.25036
403A -> 437A -0.16546
405A -> 438A 0.14765
412A -> 437A -0.12670
413A -> 438A -0.25665

416A -> 437A 0.24194
420A -> 437A 0.22662
398B -> 437B -0.21505
399B -> 438B 0.19896
400B -> 438B -0.17013
401B -> 437B 0.25039
403B -> 437B 0.16545
405B -> 438B -0.14764
412B -> 437B 0.12673
413B -> 438B 0.25676
416B -> 437B -0.24213
420B -> 437B -0.22669

Excited State 75: 3.000-A 2.3162 eV 535.30 nm f=0.0000 <S**2>=2.000
423A -> 437A 0.36038
423A -> 438A -0.25604
424A -> 437A 0.24145
424A -> 438A -0.46479
423B -> 437B -0.36586
423B -> 438B 0.26012
424B -> 437B -0.24463
424B -> 438B 0.47177

Excited State 76: 3.000-A 2.3163 eV 535.27 nm f=0.0000 <S**2>=2.000
423A -> 437A -0.23473
423A -> 438A -0.45616
424A -> 437A 0.37145
424A -> 438A 0.26174
425A -> 438A -0.10545
423B -> 437B 0.23809
423B -> 438B 0.46295
424B -> 437B -0.37702
424B -> 438B -0.26628
425B -> 438B 0.10696

Excited State 77: 1.000-A 2.3170 eV 535.11 nm f=0.0000 <S**2>=0.000

423A -> 437A -0.37370
423A -> 438A 0.23396
424A -> 437A -0.21643
424A -> 438A 0.50129
423B -> 437B -0.36820
423B -> 438B 0.23111
424B -> 437B -0.21310
424B -> 438B 0.49391

Excited State 78: 1.000-A 2.3171 eV 535.08 nm f=0.0001 <S**2>=0.000
423A -> 437A 0.21057
423A -> 438A 0.48872
424A -> 437A -0.38541
424A -> 438A -0.24144
425A -> 438A 0.11268
423B -> 437B 0.20704
423B -> 438B 0.48156
424B -> 437B -0.37978
424B -> 438B -0.23816
425B -> 438B 0.11097

Excited State 79: 3.000-A 2.3297 eV 532.19 nm f=0.0000 <S**2>=2.000
412A -> 437A -0.24552
417A -> 437A -0.48873
419A -> 438A 0.11802
420A -> 437A -0.15468
421A -> 438A -0.29727
412B -> 437B 0.24585
416B -> 437B 0.10048
417B -> 437B 0.48975
419B -> 438B -0.11833
420B -> 437B 0.15527
421B -> 438B 0.29780

Excited State 80: 3.000-A 2.3373 eV 530.46 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.11908

396A -> 438A 0.10579
398A -> 438A -0.10385
400A -> 437A -0.13455
403A -> 438A 0.10435
411A -> 437A 0.10456
412A -> 438A 0.19656
417A -> 438A 0.35339
419A -> 437A -0.36790
420A -> 438A 0.13903
421A -> 437A 0.23054
395B -> 437B -0.11906
396B -> 438B -0.10577
398B -> 438B 0.10385
400B -> 437B 0.13451
403B -> 438B -0.10433
411B -> 437B -0.10465
412B -> 438B -0.19661
417B -> 438B -0.35375
419B -> 437B 0.36857
420B -> 438B -0.13932
421B -> 437B -0.23073

Excited State 81: 1.000-A 2.3437 eV 529.00 nm f=0.0065 <S**2>=0.000
413A -> 438A -0.18682
416A -> 437A 0.33042
417A -> 437A 0.38680
419A -> 438A -0.14766
420A -> 437A 0.30687
421A -> 438A 0.25503
413B -> 438B -0.18665
416B -> 437B 0.33012
417B -> 437B 0.38572
419B -> 438B -0.14733
420B -> 437B 0.30648
421B -> 438B 0.25438

Excited State 82: 1.000-A 2.3564 eV 526.16 nm f=0.0227 <S**2>=0.000

413A -> 437A 0.26708
416A -> 438A -0.16631
417A -> 438A -0.22786
418A -> 437A 0.12894
419A -> 437A 0.48301
420A -> 438A -0.22496
421A -> 437A -0.14307
413B -> 437B 0.26701
416B -> 438B -0.16618
417B -> 438B -0.22735
418B -> 437B 0.12890
419B -> 437B 0.48255
420B -> 438B -0.22469
421B -> 437B -0.14274

Excited State 83: 1.000-A 2.3805 eV 520.84 nm f=0.0103 <S**2>=0.000

412A -> 437A 0.24676
413A -> 438A 0.25597
416A -> 437A -0.27801
417A -> 437A 0.47364
420A -> 437A -0.15478
412B -> 437B 0.24652
413B -> 438B 0.25589
416B -> 437B -0.27808
417B -> 437B 0.47353
420B -> 437B -0.15490

Excited State 84: 3.000-A 2.3888 eV 519.03 nm f=0.0000 <S**2>=2.000

433A -> 440A 0.15237
435A -> 439A 0.66043
433B -> 440B -0.15156
435B -> 439B -0.65686

Excited State 85: 1.000-A 2.3904 eV 518.67 nm f=0.0001 <S**2>=0.000

433A -> 440A 0.15482

435A -> 439A 0.68398
433B -> 440B 0.15559
435B -> 439B 0.68728

Excited State 86: 3.000-A 2.3931 eV 518.08 nm f=0.0000 <S**2>=2.000
395A -> 438A 0.29257
396A -> 437A 0.34977
397A -> 437A 0.12980
401A -> 437A -0.13859
411A -> 438A 0.13182
412A -> 437A -0.12558
415A -> 437A 0.15492
419A -> 438A -0.22223
420A -> 437A -0.17880
435A -> 439A -0.17989
395B -> 438B -0.29255
396B -> 437B -0.34977
397B -> 437B -0.12980
401B -> 437B 0.13867
411B -> 438B -0.13186
412B -> 437B 0.12578
415B -> 437B -0.15503
419B -> 438B 0.22235
420B -> 437B 0.17877
435B -> 439B 0.18039

Excited State 87: 3.000-A 2.3966 eV 517.33 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.17395
396A -> 438A -0.15009
412A -> 438A 0.11575
417A -> 438A 0.12390
419A -> 437A 0.14695
420A -> 438A 0.14857
433A -> 439A 0.13411
435A -> 440A 0.54732
395B -> 437B 0.17398

396B -> 438B 0.15011
412B -> 438B -0.11580
417B -> 438B -0.12394
419B -> 437B -0.14718
420B -> 438B -0.14877
433B -> 439B -0.13359
435B -> 440B -0.54510

Excited State 88: 3.000-A 2.3985 eV 516.93 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.23056
396A -> 438A 0.19913
411A -> 437A 0.10795
412A -> 438A -0.16220
416A -> 438A -0.11768
417A -> 438A -0.17007
419A -> 437A -0.21888
420A -> 438A -0.20509
435A -> 440A 0.40977
395B -> 437B -0.23058
396B -> 438B -0.19914
411B -> 437B -0.10811
412B -> 438B 0.16225
416B -> 438B 0.11800
417B -> 438B 0.16999
419B -> 437B 0.21949
420B -> 438B 0.20536
435B -> 440B -0.39768

Excited State 89: 1.000-A 2.3988 eV 516.87 nm f=0.0002 <S**2>=0.000
433A -> 439A 0.16295
435A -> 440A 0.67907
433B -> 439B 0.16512
435B -> 440B 0.68797

Excited State 90: 1.000-A 2.4055 eV 515.43 nm f=0.0217 <S**2>=0.000
412A -> 438A 0.10774

413A -> 437A 0.48459
416A -> 438A -0.21945
417A -> 438A 0.22757
419A -> 437A -0.29828
420A -> 438A -0.10250
412B -> 438B 0.10786
413B -> 437B 0.48463
416B -> 438B -0.21926
417B -> 438B 0.22773
419B -> 437B -0.29801
420B -> 438B -0.10219

Excited State 91: 1.000-A 2.4310 eV 510.01 nm f=0.0010 <S**2>=0.000
411A -> 437A -0.10480
412A -> 438A 0.27156
416A -> 438A 0.14111
417A -> 438A 0.38198
418A -> 437A 0.17151
419A -> 437A 0.27387
420A -> 438A 0.32533
411B -> 437B -0.10453
412B -> 438B 0.27179
416B -> 438B 0.14131
417B -> 438B 0.38224
418B -> 437B 0.17237
419B -> 437B 0.27510
420B -> 438B 0.32568

Excited State 92: 3.000-A 2.4356 eV 509.04 nm f=0.0000 <S**2>=2.000
394A -> 437A -0.10143
395A -> 437A 0.24525
396A -> 438A 0.21463
403A -> 438A -0.10487
412A -> 438A 0.11105
413A -> 437A -0.10429
414A -> 437A 0.19638

415A -> 438A 0.10142
417A -> 438A 0.11131
418A -> 437A 0.24299
419A -> 437A 0.38607
420A -> 438A 0.13887
394B -> 437B 0.10146
395B -> 437B -0.24533
396B -> 438B -0.21469
403B -> 438B 0.10504
412B -> 438B -0.11008
413B -> 437B 0.10453
414B -> 437B -0.19642
415B -> 438B -0.10165
417B -> 438B -0.11003
418B -> 437B -0.24235
419B -> 437B -0.38494
420B -> 438B -0.13769

Excited State 93: 1.000-A 2.4513 eV 505.79 nm f=0.0024 <S**2>=0.000
403A -> 437A 0.10108
411A -> 438A -0.11874
412A -> 437A 0.36129
413A -> 438A 0.13997
416A -> 437A 0.10622
417A -> 437A -0.12130
418A -> 438A 0.21253
419A -> 438A 0.42121
420A -> 437A 0.17914
403B -> 437B 0.10087
411B -> 438B -0.11869
412B -> 437B 0.36187
413B -> 438B 0.14006
416B -> 437B 0.10653
417B -> 437B -0.12184
418B -> 438B 0.21299
419B -> 438B 0.42161

420B -> 437B 0.17953

Excited State 94: 3.000-A 2.4602 eV 503.97 nm f=0.0000 <S**2>=2.000

395A -> 438A 0.11111
396A -> 437A 0.13159
398A -> 437A -0.10221
412A -> 437A 0.30913
414A -> 438A 0.15078
415A -> 437A 0.24254
416A -> 437A 0.15824
417A -> 437A -0.27362
418A -> 438A 0.21923
419A -> 438A 0.21067
420A -> 437A 0.22564
395B -> 438B -0.11114
396B -> 437B -0.13161
398B -> 437B 0.10236
412B -> 437B -0.30857
414B -> 438B -0.15099
415B -> 437B -0.24311
416B -> 437B -0.15793
417B -> 437B 0.27341
418B -> 438B -0.21883
419B -> 438B -0.20971
420B -> 437B -0.22532

Excited State 95: 3.000-A 2.4753 eV 500.88 nm f=0.0000 <S**2>=2.000

398A -> 437A -0.14782
399A -> 438A 0.13227
403A -> 437A 0.11412
411A -> 438A 0.24233
412A -> 437A 0.10944
413A -> 438A -0.13546
414A -> 438A -0.14057
415A -> 437A -0.14002
417A -> 437A -0.32864

419A -> 438A -0.34359
421A -> 438A 0.10598
398B -> 437B 0.14783
399B -> 438B -0.13228
403B -> 437B -0.11420
411B -> 438B -0.24243
412B -> 437B -0.10961
413B -> 438B 0.13545
414B -> 438B 0.14082
415B -> 437B 0.14048
417B -> 437B 0.32869
419B -> 438B 0.34375
421B -> 438B -0.10598

Excited State 96: 3.000-A 2.4786 eV 500.23 nm f=0.0000 <S**2>=2.000
398A -> 438A -0.12213
399A -> 437A 0.13471
411A -> 437A 0.27846
413A -> 437A -0.27204
414A -> 437A -0.36379
414A -> 440A -0.17662
415A -> 438A -0.20006
415A -> 439A 0.17156
398B -> 438B 0.12215
399B -> 437B -0.13477
411B -> 437B -0.27876
413B -> 437B 0.27199
414B -> 437B 0.36489
414B -> 440B 0.17664
415B -> 438B 0.20069
415B -> 439B -0.17158

Excited State 97: 1.000-A 2.4837 eV 499.19 nm f=0.0005 <S**2>=0.000
412A -> 437A 0.11577
414A -> 438A 0.32799
415A -> 437A 0.58339

412B -> 437B 0.11567
414B -> 438B 0.32838
415B -> 437B 0.58436

Excited State 98: 1.000-A 2.4864 eV 498.65 nm f=0.0011 <S**2>=0.000
414A -> 437A 0.60351
415A -> 438A 0.33857
414B -> 437B 0.60332
415B -> 438B 0.33840

Excited State 99: 3.000-A 2.4876 eV 498.42 nm f=0.0000 <S**2>=2.000
395A -> 438A -0.14432
396A -> 437A -0.17273
414A -> 438A 0.17764
414A -> 439A -0.29581
415A -> 437A 0.34453
415A -> 440A 0.28587
416A -> 437A -0.13281
418A -> 438A -0.12756
419A -> 438A -0.19974
395B -> 438B 0.14433
396B -> 437B 0.17275
414B -> 438B -0.17659
414B -> 439B 0.29579
415B -> 437B -0.34275
415B -> 440B -0.28585
416B -> 437B 0.13256
418B -> 438B 0.12766
419B -> 438B 0.19969

Excited State 100: 3.000-A 2.4921 eV 497.51 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.14336
396A -> 438A -0.12592
399A -> 437A 0.10122
403A -> 438A 0.10161
411A -> 437A 0.22240

413A -> 437A -0.28611
414A -> 437A 0.20481
414A -> 440A 0.26458
415A -> 438A 0.11670
415A -> 439A -0.25721
418A -> 437A -0.12016
420A -> 438A -0.15079
395B -> 437B 0.14334
396B -> 438B 0.12590
399B -> 437B -0.10125
403B -> 438B -0.10163
411B -> 437B -0.22271
413B -> 437B 0.28617
414B -> 437B -0.20400
414B -> 440B -0.26458
415B -> 438B -0.11619
415B -> 439B 0.25721
418B -> 437B 0.12014
420B -> 438B 0.15105

Excited State 101: 1.000-A 2.5109 eV 493.79 nm f=0.0098 <S**2>=0.000
399A -> 437A 0.10226
400A -> 437A 0.10911
403A -> 438A -0.12858
411A -> 437A 0.35714
413A -> 437A -0.26231
417A -> 438A 0.31283
419A -> 437A 0.16064
420A -> 438A -0.26141
399B -> 437B 0.10205
400B -> 437B 0.10924
403B -> 438B -0.12873
411B -> 437B 0.35669
413B -> 437B -0.26211
417B -> 438B 0.31354
419B -> 437B 0.16068

420B -> 438B -0.26183

Excited State 102: 3.000-A 2.5143 eV 493.11 nm f=0.0000 <S**2>=2.000
414A -> 438A -0.16180
414A -> 439A -0.34240
415A -> 437A -0.33660
415A -> 440A 0.33787
416A -> 437A 0.11767
416A -> 440A -0.10409
419A -> 438A 0.14517
414B -> 438B 0.16161
414B -> 439B 0.34242
415B -> 437B 0.33630
415B -> 440B -0.33787
416B -> 437B -0.11766
416B -> 440B 0.10408
419B -> 438B -0.14537

Excited State 103: 3.000-A 2.5145 eV 493.08 nm f=0.0000 <S**2>=2.000
413A -> 437A -0.10538
414A -> 437A 0.32953
414A -> 440A -0.31742
415A -> 438A 0.15099
415A -> 439A 0.30336
417A -> 438A 0.13468
418A -> 437A -0.16952
420A -> 438A -0.17206
434A -> 439A 0.15414
413B -> 437B 0.10502
414B -> 437B -0.32931
414B -> 440B 0.31742
415B -> 438B -0.15090
415B -> 439B -0.30339
417B -> 438B -0.13443
418B -> 437B 0.16967
420B -> 438B 0.17197

434B -> 439B -0.15415

Excited State 104: 1.000-A 2.5174 eV 492.50 nm f=0.0038 <S**2>=0.000
412A -> 437A -0.23492
413A -> 438A -0.19097
415A -> 437A 0.11904
417A -> 437A 0.28256
418A -> 438A -0.14158
419A -> 438A 0.47620
420A -> 437A -0.16584
421A -> 438A -0.11241
412B -> 437B -0.23472
413B -> 438B -0.19144
415B -> 437B 0.11938
417B -> 437B 0.28249
418B -> 438B -0.14189
419B -> 438B 0.47650
420B -> 437B -0.16604
421B -> 438B -0.11250

Excited State 105: 3.000-A 2.5211 eV 491.79 nm f=0.0000 <S**2>=2.000
411A -> 437A 0.12361
414A -> 437A 0.16987
415A -> 438A 0.11262
417A -> 438A -0.44012
418A -> 437A 0.14867
419A -> 437A -0.11805
420A -> 438A 0.35169
411B -> 437B -0.12461
414B -> 437B -0.16970
415B -> 438B -0.11249
417B -> 438B 0.44030
418B -> 437B -0.14921
419B -> 437B 0.11796
420B -> 438B -0.35211

Excited State 106: 3.000-A 2.5266 eV 490.71 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 414A -> 440A | -0.11356 |
| 415A -> 439A | 0.10972 |
| 431A -> 440A | 0.17284 |
| 434A -> 439A | -0.63475 |
| 414B -> 440B | 0.11356 |
| 415B -> 439B | -0.10973 |
| 431B -> 440B | -0.17285 |
| 434B -> 439B | 0.63476 |

Excited State 107: 3.000-A 2.5279 eV 490.47 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 409A -> 437A | -0.12117 |
| 411A -> 438A | 0.14032 |
| 413A -> 438A | -0.36469 |
| 415A -> 437A | 0.14230 |
| 418A -> 438A | -0.23827 |
| 419A -> 438A | 0.34075 |
| 420A -> 437A | -0.21939 |
| 421A -> 438A | -0.11537 |
| 409B -> 437B | 0.12126 |
| 411B -> 438B | -0.14057 |
| 413B -> 438B | 0.36472 |
| 415B -> 437B | -0.14213 |
| 418B -> 438B | 0.23825 |
| 419B -> 438B | -0.34014 |
| 420B -> 437B | 0.21927 |
| 421B -> 438B | 0.11529 |

Excited State 108: 1.000-A 2.5287 eV 490.31 nm f=0.0066 <S**2>=0.000

| | |
|---|---|
| 398A -> 438A | -0.13536 |
| 399A -> 437A | 0.11447 |
| 400A -> 437A | 0.17051 |
| 403A -> 438A | -0.17137 |
| 411A -> 437A | 0.31092 |
| 417A -> 438A | -0.25310 |
| 418A -> 437A | 0.30226 |

420A -> 438A 0.34562
398B -> 438B -0.13516
399B -> 437B 0.11435
400B -> 437B 0.17059
403B -> 438B -0.17147
411B -> 437B 0.31067
417B -> 438B -0.25212
418B -> 437B 0.30180
420B -> 438B 0.34484

Excited State 109: 3.000-A 2.5378 eV 488.55 nm f=0.0000 <S**2>=2.000
431A -> 439A 0.19371
434A -> 440A -0.64837
431B -> 439B -0.19371
434B -> 440B 0.64838

Excited State 110: 1.000-A 2.5387 eV 488.37 nm f=0.0019 <S**2>=0.000
431A -> 440A -0.16746
434A -> 439A 0.67421
431B -> 440B -0.16746
434B -> 439B 0.67420

Excited State 111: 1.000-A 2.5487 eV 486.45 nm f=0.0005 <S**2>=0.000
431A -> 439A -0.17678
434A -> 440A 0.66265
431B -> 439B -0.17678
434B -> 440B 0.66265

Excited State 112: 1.000-A 2.5489 eV 486.42 nm f=0.0039 <S**2>=0.000
398A -> 437A 0.15381
399A -> 438A -0.13323
400A -> 438A -0.16731
403A -> 437A 0.26739
409A -> 437A 0.16537
411A -> 438A -0.28432
412A -> 437A -0.26797

413A -> 438A 0.29693
434A -> 440A -0.11050
398B -> 437B 0.15368
399B -> 438B -0.13313
400B -> 438B -0.16734
403B -> 437B 0.26744
409B -> 437B 0.16525
411B -> 438B -0.28413
412B -> 437B -0.26790
413B -> 438B 0.29671
434B -> 440B -0.11048

Excited State 113: 1.000-A 2.5584 eV 484.61 nm f=0.0006 <S**2>=0.000
398A -> 437A -0.13557
400A -> 438A 0.16766
403A -> 437A -0.27563
412A -> 437A -0.34048
413A -> 438A 0.18781
418A -> 438A 0.37365
419A -> 438A 0.10229
420A -> 437A 0.16249
398B -> 437B -0.13563
400B -> 438B 0.16754
403B -> 437B -0.27549
412B -> 437B -0.34069
413B -> 438B 0.18758
418B -> 438B 0.37381
419B -> 438B 0.10242
420B -> 437B 0.16254

Excited State 114: 3.000-A 2.5625 eV 483.84 nm f=0.0000 <S**2>=2.000
431A -> 443A 0.15594
434A -> 444A 0.26418
436A -> 443A -0.57790
431B -> 443B -0.15594
434B -> 444B -0.26418

436B -> 443B 0.57790

Excited State 115: 3.000-A 2.5720 eV 482.06 nm f=0.0000 <S**2>=2.000
409A -> 437A 0.19839
410A -> 438A -0.12435
411A -> 438A -0.17825
412A -> 437A 0.22354
413A -> 438A 0.21527
416A -> 437A 0.28222
418A -> 438A -0.41548
420A -> 437A -0.15128
409B -> 437B -0.19906
410B -> 438B 0.12448
411B -> 438B 0.17847
412B -> 437B -0.22341
413B -> 438B -0.21656
416B -> 437B -0.28345
418B -> 438B 0.41638
420B -> 437B 0.15149

Excited State 116: 1.000-A 2.5786 eV 480.82 nm f=0.0001 <S**2>=0.000
400A -> 438A 0.11989
403A -> 437A -0.22115
409A -> 437A 0.17510
413A -> 438A 0.33252
416A -> 437A 0.35558
418A -> 438A -0.33715
400B -> 438B 0.11971
403B -> 437B -0.22088
409B -> 437B 0.17432
413B -> 438B 0.33192
416B -> 437B 0.35469
418B -> 438B -0.33578

Excited State 117: 3.000-A 2.5819 eV 480.21 nm f=0.0000 <S**2>=2.000
410A -> 437A 0.12652

412A -> 438A -0.13602
413A -> 437A -0.20301
415A -> 438A -0.11868
416A -> 438A -0.48187
417A -> 438A 0.13105
418A -> 437A 0.26716
420A -> 438A 0.14351
410B -> 437B -0.12666
412B -> 438B 0.13631
413B -> 437B 0.20403
415B -> 438B 0.11927
416B -> 438B 0.48397
417B -> 438B -0.13143
418B -> 437B -0.26812
420B -> 438B -0.14376

Excited State 118: 1.000-A 2.5870 eV 479.25 nm f=0.0006 <S**2>=0.000
411A -> 437A 0.29172
413A -> 437A 0.24319
415A -> 438A 0.13845
416A -> 438A 0.48870
418A -> 437A -0.23990
411B -> 437B 0.29341
413B -> 437B 0.24331
415B -> 438B 0.13838
416B -> 438B 0.48794
418B -> 437B -0.23913

Excited State 119: 3.000-A 2.5891 eV 478.87 nm f=0.0000 <S**2>=2.000
410A -> 437A 0.14428
411A -> 437A 0.21381
412A -> 438A -0.17468
413A -> 437A 0.12643
416A -> 438A 0.17552
431A -> 444A -0.12822
434A -> 443A -0.25941

436A -> 442A 0.14441
436A -> 444A 0.41584
410B -> 437B -0.14451
411B -> 437B -0.21219
412B -> 438B 0.17523
413B -> 437B -0.12494
416B -> 438B -0.17249
431B -> 444B 0.12822
434B -> 443B 0.25941
436B -> 442B -0.14437
436B -> 444B -0.41584

Excited State 120: 3.000-A 2.5932 eV 478.11 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.16967
410A -> 438A 0.16508
411A -> 438A 0.25344
412A -> 437A -0.32640
413A -> 438A 0.34600
415A -> 437A 0.10968
416A -> 437A 0.27158
418A -> 438A -0.12248
419A -> 438A 0.10534
409B -> 437B 0.17007
410B -> 438B -0.16525
411B -> 438B -0.25376
412B -> 437B 0.32631
413B -> 438B -0.34595
415B -> 437B -0.10973
416B -> 437B -0.27149
418B -> 438B 0.12251
419B -> 438B -0.10526

Excited State 121: 3.000-A 2.5935 eV 478.07 nm f=0.0000 <S**2>=2.000
410A -> 437A 0.28503
411A -> 437A 0.28287
412A -> 438A -0.29886

413A -> 437A 0.10892
416A -> 438A 0.10187
417A -> 438A 0.11539
434A -> 443A 0.17474
436A -> 444A -0.28649
410B -> 437B -0.28579
411B -> 437B -0.28289
412B -> 438B 0.29927
413B -> 437B -0.10846
416B -> 438B -0.10080
417B -> 438B -0.11560
434B -> 443B -0.17474
436B -> 444B 0.28651

Excited State 122: 1.000-A 2.5997 eV 476.91 nm f=0.0070 <S**2>=0.000
398A -> 438A -0.15453
399A -> 437A 0.17617
400A -> 437A 0.33789
403A -> 438A -0.29754
409A -> 438A 0.15317
410A -> 437A -0.23193
411A -> 437A -0.27055
416A -> 438A 0.15879
398B -> 438B -0.15431
399B -> 437B 0.17600
400B -> 437B 0.33776
403B -> 438B -0.29747
409B -> 438B 0.15295
410B -> 437B -0.23113
411B -> 437B -0.26972
416B -> 438B 0.15886

Excited State 123: 1.000-A 2.6137 eV 474.36 nm f=0.0184 <S**2>=0.000
410A -> 437A -0.29373
412A -> 438A 0.55253
416A -> 438A -0.10238

417A -> 438A -0.20288
410B -> 437B -0.29348
412B -> 438B 0.55215
416B -> 438B -0.10231
417B -> 438B -0.20273

Excited State 124: 1.000-A 2.6227 eV 472.73 nm f=0.0054 <S**2>=0.000
400A -> 438A 0.11454
403A -> 437A -0.17060
409A -> 437A 0.40277
410A -> 438A -0.24824
411A -> 438A -0.31903
413A -> 438A -0.21904
416A -> 437A -0.13443
418A -> 438A 0.15104
400B -> 438B 0.11443
403B -> 437B -0.17048
409B -> 437B 0.40279
410B -> 438B -0.24817
411B -> 438B -0.31875
413B -> 438B -0.21881
416B -> 437B -0.13425
418B -> 438B 0.15105

Excited State 125: 1.000-A 2.6421 eV 469.26 nm f=0.0000 <S**2>=0.000
399A -> 437A 0.15045
400A -> 437A 0.14244
401A -> 438A 0.10727
403A -> 438A -0.10008
404A -> 437A -0.16075
405A -> 437A -0.14447
408A -> 437A 0.17660
409A -> 438A -0.16042
410A -> 437A 0.38508
411A -> 437A -0.16293
412A -> 438A 0.22593

413A -> 437A -0.11347
417A -> 438A -0.12117
418A -> 437A -0.11145
399B -> 437B 0.14994
400B -> 437B 0.14336
401B -> 438B 0.10745
403B -> 438B -0.10072
404B -> 437B -0.16115
405B -> 437B -0.14487
408B -> 437B 0.17850
409B -> 438B -0.16242
410B -> 437B 0.38838
411B -> 437B -0.16406
412B -> 438B 0.22825
413B -> 437B -0.11444
417B -> 438B -0.12220
418B -> 437B -0.11249

Excited State 126: 3.000-A 2.6456 eV 468.64 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.11268
408A -> 437A 0.24765
409A -> 438A -0.25111
410A -> 437A 0.39916
411A -> 437A -0.13095
412A -> 438A 0.27796
413A -> 437A -0.11879
417A -> 438A -0.12193
418A -> 437A -0.12621
400B -> 437B -0.11158
408B -> 437B -0.24630
409B -> 438B 0.24984
410B -> 437B -0.39596
411B -> 437B 0.12959
412B -> 438B -0.27617
413B -> 437B 0.11785
417B -> 438B 0.12096

418B -> 437B 0.12531

Excited State 127: 3.000-A 2.6518 eV 467.55 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.17925
401A -> 437A 0.18858
403A -> 437A -0.16396
405A -> 438A -0.12593
407A -> 437A 0.23471
408A -> 438A 0.20360
409A -> 437A -0.37022
410A -> 438A 0.25152
418A -> 438A -0.14231
419A -> 438A -0.10871
398B -> 437B -0.17925
401B -> 437B -0.18896
403B -> 437B 0.16430
405B -> 438B 0.12610
407B -> 437B -0.23528
408B -> 438B -0.20390
409B -> 437B 0.37038
410B -> 438B -0.25171
418B -> 438B 0.14234
419B -> 438B 0.10882

Excited State 128: 3.000-A 2.6590 eV 466.28 nm f=0.0000 <S**2>=2.000
404A -> 437A -0.36943
405A -> 437A 0.27684
408A -> 437A -0.36103
410A -> 437A 0.26148
411A -> 437A -0.23684
404B -> 437B 0.37112
405B -> 437B -0.27796
408B -> 437B 0.36290
410B -> 437B -0.26202
411B -> 437B 0.23738

Excited State 129: 3.000-A 2.6599 eV 466.13 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 398A -> 437A | -0.19553 |
| 401A -> 437A | -0.12822 |
| 402A -> 438A | -0.17672 |
| 403A -> 437A | 0.14371 |
| 404A -> 438A | 0.21656 |
| 407A -> 437A | -0.20911 |
| 409A -> 437A | -0.34255 |
| 411A -> 438A | -0.32058 |
| 414A -> 438A | 0.16228 |
| 398B -> 437B | 0.19575 |
| 401B -> 437B | 0.12897 |
| 402B -> 438B | 0.17719 |
| 403B -> 437B | -0.14373 |
| 404B -> 438B | -0.21734 |
| 407B -> 437B | 0.20982 |
| 409B -> 437B | 0.34331 |
| 411B -> 438B | 0.32144 |
| 414B -> 438B | -0.16280 |

Excited State 130: 1.000-A 2.6680 eV 464.71 nm f=0.0034 <S**2>=0.000

| | |
|---|---|
| 402A -> 437A | -0.12568 |
| 404A -> 437A | 0.42567 |
| 405A -> 437A | -0.18965 |
| 408A -> 437A | 0.41576 |
| 409A -> 438A | -0.15037 |
| 410A -> 437A | -0.13897 |
| 411A -> 437A | 0.12684 |
| 402B -> 437B | -0.12552 |
| 404B -> 437B | 0.42462 |
| 405B -> 437B | -0.18833 |
| 408B -> 437B | 0.41415 |
| 409B -> 438B | -0.15041 |
| 410B -> 437B | -0.13775 |
| 411B -> 437B | 0.12564 |

Excited State 131: 1.000-A 2.6683 eV 464.66 nm f=0.0191 <S**2>=0.000

| | |
|---|---|
| 396A -> 437A | -0.10197 |
| 399A -> 438A | 0.11668 |
| 401A -> 437A | 0.30207 |
| 403A -> 437A | -0.12973 |
| 404A -> 438A | -0.14489 |
| 405A -> 438A | -0.11250 |
| 406A -> 437A | -0.22194 |
| 407A -> 437A | 0.36318 |
| 408A -> 438A | 0.13910 |
| 410A -> 438A | 0.20584 |
| 413A -> 438A | -0.14480 |
| 435A -> 441A | -0.10647 |
| 396B -> 437B | -0.10210 |
| 399B -> 438B | 0.11691 |
| 401B -> 437B | 0.30159 |
| 403B -> 437B | -0.12929 |
| 404B -> 438B | -0.14443 |
| 405B -> 438B | -0.11228 |
| 406B -> 437B | -0.22180 |
| 407B -> 437B | 0.36257 |
| 408B -> 438B | 0.13893 |
| 410B -> 438B | 0.20546 |
| 413B -> 438B | -0.14471 |
| 435B -> 441B | -0.10646 |

Excited State 132: 1.000-A 2.6714 eV 464.12 nm f=0.0001 <S**2>=0.000

| | |
|---|---|
| 400A -> 438A | -0.10558 |
| 402A -> 438A | 0.15799 |
| 404A -> 438A | -0.22061 |
| 408A -> 438A | -0.16719 |
| 409A -> 437A | 0.38690 |
| 411A -> 438A | 0.36386 |
| 414A -> 438A | -0.19166 |
| 415A -> 437A | 0.12575 |
| 419A -> 438A | 0.10704 |

400B -> 438B -0.10548
402B -> 438B 0.15753
404B -> 438B -0.22016
408B -> 438B -0.16688
409B -> 437B 0.38591
411B -> 438B 0.36309
414B -> 438B -0.19125
415B -> 437B 0.12550
419B -> 438B 0.10676

Excited State 133: 3.000-A 2.6745 eV 463.58 nm f=0.0000 <S**2>=2.000
398A -> 438A -0.21445
399A -> 437A 0.15922
401A -> 438A -0.12952
402A -> 437A -0.13715
403A -> 438A 0.13915
404A -> 437A 0.34258
405A -> 437A 0.14437
407A -> 438A -0.15827
409A -> 438A -0.22854
410A -> 437A 0.13815
411A -> 437A -0.17381
412A -> 438A -0.23422
415A -> 438A -0.13407
398B -> 438B 0.21442
399B -> 437B -0.15905
401B -> 438B 0.12985
402B -> 437B 0.13718
403B -> 438B -0.13913
404B -> 437B -0.34247
405B -> 437B -0.14535
407B -> 438B 0.15850
409B -> 438B 0.22883
410B -> 437B -0.13889
411B -> 437B 0.17425
412B -> 438B 0.23408

415B -> 438B 0.13417

Excited State 134: 1.000-A 2.6850 eV 461.77 nm f=0.0078 <S**2>=0.000
395A -> 437A 0.10048
399A -> 437A -0.13548
401A -> 438A -0.17521
404A -> 437A 0.24299
405A -> 437A 0.40569
409A -> 438A -0.24177
410A -> 437A 0.24578
411A -> 437A -0.14018
433A -> 441A -0.10023
435A -> 442A 0.13607
395B -> 437B 0.10048
399B -> 437B -0.13573
401B -> 438B -0.17487
404B -> 437B 0.24273
405B -> 437B 0.40544
409B -> 438B -0.24129
410B -> 437B 0.24544
411B -> 437B -0.13971
433B -> 441B -0.10021
435B -> 442B 0.13605

Excited State 135: 2.993-A 2.6920 eV 460.57 nm f=0.0000 <S**2>=1.990
404A -> 437A -0.17368
405A -> 437A -0.10469
414A -> 437A 0.28740
415A -> 438A -0.50438
416A -> 438A 0.12971
404B -> 437B 0.18393
405B -> 437B 0.10859
414B -> 437B -0.33393
415B -> 438B 0.58534
416B -> 438B -0.15140

Excited State 136: 1.020-A 2.6921 eV 460.55 nm f=0.0000 <S**2>=0.010

| | |
|---|---|
| 414A -> 437A | -0.35015 |
| 415A -> 438A | 0.60878 |
| 416A -> 438A | -0.16300 |
| 414B -> 437B | -0.30603 |
| 415B -> 438B | 0.53148 |
| 416B -> 438B | -0.14305 |

Excited State 137: 3.000-A 2.6958 eV 459.91 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 431A -> 440A | 0.11303 |
| 432A -> 439A | 0.29891 |
| 433A -> 439A | 0.59179 |
| 435A -> 440A | -0.14815 |
| 431B -> 440B | -0.11301 |
| 432B -> 439B | -0.29887 |
| 433B -> 439B | -0.59163 |
| 435B -> 440B | 0.14812 |

Excited State 138: 1.018-A 2.6962 eV 459.85 nm f=0.0030 <S**2>=0.009

| | |
|---|---|
| 401A -> 437A | 0.11707 |
| 404A -> 438A | -0.16112 |
| 409A -> 437A | 0.11952 |
| 414A -> 438A | 0.49972 |
| 415A -> 437A | -0.25506 |
| 401B -> 437B | 0.12368 |
| 404B -> 438B | -0.18266 |
| 405B -> 438B | -0.10517 |
| 407B -> 437B | -0.10971 |
| 409B -> 437B | 0.13291 |
| 414B -> 438B | 0.57535 |
| 415B -> 437B | -0.29430 |

Excited State 139: 2.994-A 2.6963 eV 459.82 nm f=0.0000 <S**2>=1.991

| | |
|---|---|
| 404A -> 438A | -0.16971 |
| 409A -> 437A | 0.10744 |
| 411A -> 438A | 0.12233 |

414A -> 438A 0.59332
415A -> 437A -0.30785
404B -> 438B 0.14638
411B -> 438B -0.11229
414B -> 438B -0.52043
415B -> 437B 0.27058

Excited State 140: 1.000-A 2.7032 eV 458.65 nm f=0.0002 <S**2>=0.000
432A -> 439A 0.19076
433A -> 439A 0.65244
435A -> 440A -0.15961
432B -> 439B 0.19084
433B -> 439B 0.65257
435B -> 440B -0.15965

Excited State 141: 3.000-A 2.7064 eV 458.11 nm f=0.0000 <S**2>=2.000
431A -> 439A 0.10725
432A -> 440A 0.26321
433A -> 440A 0.60332
435A -> 439A -0.14092
431B -> 439B -0.10723
432B -> 440B -0.26315
433B -> 440B -0.60309
435B -> 439B 0.14087

Excited State 142: 3.000-A 2.7078 eV 457.88 nm f=0.0000 <S**2>=2.000
401A -> 437A 0.10870
402A -> 438A -0.14338
405A -> 438A -0.34174
406A -> 437A 0.32582
407A -> 437A -0.30517
408A -> 438A 0.10816
410A -> 438A -0.10304
411A -> 438A 0.16916
412A -> 437A 0.12729
414A -> 438A -0.15860

433A -> 440A -0.11766
401B -> 437B -0.10946
402B -> 438B 0.14394
405B -> 438B 0.34289
406B -> 437B -0.32570
407B -> 437B 0.30699
408B -> 438B -0.10793
410B -> 438B 0.10275
411B -> 438B -0.16858
412B -> 437B -0.12744
414B -> 438B 0.15936
433B -> 440B 0.11789

Excited State 143: 1.000-A 2.7104 eV 457.44 nm f=0.0075 <S**2>=0.000
398A -> 437A 0.17503
399A -> 438A -0.10776
401A -> 437A -0.10724
402A -> 438A 0.10312
405A -> 438A 0.19519
406A -> 437A 0.14723
407A -> 437A 0.46220
408A -> 438A 0.13815
410A -> 438A -0.11568
411A -> 438A 0.16600
414A -> 438A 0.18224
415A -> 437A -0.11073
433A -> 440A 0.12740
398B -> 437B 0.17490
399B -> 438B -0.10666
401B -> 437B -0.10642
402B -> 438B 0.10304
405B -> 438B 0.19426
406B -> 437B 0.15190
407B -> 437B 0.46661
408B -> 438B 0.14226
410B -> 438B -0.12068

411B -> 438B 0.16945
414B -> 438B 0.18288
415B -> 437B -0.11116
433B -> 440B 0.12756

Excited State 144: 3.000-A 2.7116 eV 457.24 nm f=0.0000 <S**2>=2.000
404A -> 438A 0.34021
406A -> 437A 0.20605
407A -> 437A 0.36198
408A -> 438A 0.23405
410A -> 438A -0.29178
411A -> 438A 0.18556
404B -> 438B -0.33970
406B -> 437B -0.20454
407B -> 437B -0.35562
408B -> 438B -0.23243
410B -> 438B 0.29056
411B -> 438B -0.18353

Excited State 145: 1.000-A 2.7120 eV 457.17 nm f=0.0004 <S**2>=0.000
432A -> 440A 0.17677
433A -> 440A 0.64424
435A -> 439A -0.14792
432B -> 440B 0.17690
433B -> 440B 0.64455
435B -> 439B -0.14801

Excited State 146: 1.001-A 2.7227 eV 455.38 nm f=0.0028 <S**2>=0.000
402A -> 437A 0.18987
404A -> 437A -0.25886
405A -> 437A 0.29399
407A -> 438A 0.31563
408A -> 437A 0.38938
402B -> 437B 0.19489
404B -> 437B -0.26026
405B -> 437B 0.30385

407B -> 438B 0.32377
408B -> 437B 0.39798

Excited State 147: 3.000-A 2.7237 eV 455.21 nm f=0.0000 <S**2>=2.000
402A -> 437A 0.21066
405A -> 437A 0.40333
407A -> 438A 0.34166
408A -> 437A 0.34966
412A -> 438A -0.11054
415A -> 438A -0.11404
402B -> 437B -0.20604
405B -> 437B -0.39607
407B -> 438B -0.33390
408B -> 437B -0.34005
412B -> 438B 0.10951
415B -> 438B 0.11229

Excited State 148: 1.000-A 2.7247 eV 455.04 nm f=0.0018 <S**2>=0.000
399A -> 438A 0.10655
401A -> 437A 0.22254
402A -> 438A -0.12011
404A -> 438A 0.12808
405A -> 438A -0.25864
406A -> 437A 0.41453
408A -> 438A 0.23506
410A -> 438A -0.23023
411A -> 438A 0.12548
399B -> 438B 0.10655
401B -> 437B 0.22239
402B -> 438B -0.11997
404B -> 438B 0.12755
405B -> 438B -0.25821
406B -> 437B 0.41408
408B -> 438B 0.23467
410B -> 438B -0.22979
411B -> 438B 0.12505

Excited State 149: 3.000-A 2.7390 eV 452.66 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 431A -> 444A | -0.12019 |
| 432A -> 439A | 0.18591 |
| 432A -> 448A | 0.11650 |
| 433A -> 439A | -0.18374 |
| 434A -> 443A | -0.15308 |
| 436A -> 442A | -0.28425 |
| 436A -> 445A | 0.11750 |
| 436A -> 446A | 0.34178 |
| 436A -> 453A | -0.11701 |
| 436A -> 464A | 0.11060 |
| 431B -> 444B | 0.12019 |
| 432B -> 439B | -0.18591 |
| 432B -> 448B | -0.11650 |
| 433B -> 439B | 0.18375 |
| 434B -> 443B | 0.15308 |
| 436B -> 442B | 0.28423 |
| 436B -> 445B | -0.11751 |
| 436B -> 446B | -0.34178 |
| 436B -> 453B | 0.11700 |
| 436B -> 464B | -0.11060 |

Excited State 150: 3.000-A 2.7391 eV 452.65 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 398A -> 437A | 0.10719 |
| 401A -> 437A | 0.14440 |
| 403A -> 437A | -0.13033 |
| 404A -> 438A | 0.40052 |
| 405A -> 438A | -0.11791 |
| 406A -> 437A | -0.42637 |
| 407A -> 437A | -0.22334 |
| 411A -> 438A | 0.12922 |
| 398B -> 437B | -0.10739 |
| 401B -> 437B | -0.14473 |
| 403B -> 437B | 0.13051 |
| 404B -> 438B | -0.40153 |

405B -> 438B 0.11810
406B -> 437B 0.42695
407B -> 437B 0.22338
411B -> 438B -0.12974

Excited State 151: 3.000-A 2.7432 eV 451.97 nm f=0.0000 <S**2>=2.000
398A -> 438A -0.14536
401A -> 438A -0.21555
402A -> 437A -0.10701
403A -> 438A 0.20971
404A -> 437A -0.34095
406A -> 438A 0.25859
407A -> 438A -0.12954
408A -> 437A 0.23689
409A -> 438A -0.15155
410A -> 437A -0.15241
415A -> 438A 0.12793
398B -> 438B 0.14542
401B -> 438B 0.21609
402B -> 437B 0.10768
403B -> 438B -0.21004
404B -> 437B 0.34161
406B -> 438B -0.25925
407B -> 438B 0.13032
408B -> 437B -0.23695
409B -> 438B 0.15201
410B -> 437B 0.15270
415B -> 438B -0.12822

Excited State 152: 1.000-A 2.7528 eV 450.39 nm f=0.0021 <S**2>=0.000
399A -> 437A -0.17380
400A -> 437A 0.12377
401A -> 438A -0.13586
402A -> 437A -0.14480
404A -> 437A -0.20382
404A -> 438A 0.36154

406A -> 437A -0.28388
406A -> 438A 0.17403
407A -> 438A -0.15507
410A -> 438A -0.11978
411A -> 438A 0.16004
399B -> 437B -0.17368
400B -> 437B 0.12361
401B -> 438B -0.13548
402B -> 437B -0.14458
404B -> 437B -0.20320
404B -> 438B 0.36086
406B -> 437B -0.28325
406B -> 438B 0.17355
407B -> 438B -0.15476
410B -> 438B -0.11968
411B -> 438B 0.15984

Excited State 153: 1.000-A 2.7528 eV 450.39 nm f=0.0026 <S**2>=0.000
399A -> 437A 0.19311
400A -> 437A -0.13773
401A -> 438A 0.15073
402A -> 437A 0.16151
404A -> 437A 0.22665
404A -> 438A 0.32438
406A -> 437A -0.25531
406A -> 438A -0.19456
407A -> 438A 0.17349
409A -> 438A 0.10215
410A -> 438A -0.10746
411A -> 438A 0.14395
399B -> 437B 0.19298
400B -> 437B -0.13756
401B -> 438B 0.15031
402B -> 437B 0.16126
404B -> 437B 0.22598
404B -> 438B 0.32379

406B -> 437B -0.25477
406B -> 438B -0.19404
407B -> 438B 0.17315
409B -> 438B 0.10187
410B -> 438B -0.10738
411B -> 438B 0.14377

Excited State 154: 3.000-A 2.7554 eV 449.97 nm f=0.0000 <S**2>=2.000
430A -> 440A 0.11131
431A -> 440A -0.18579
432A -> 439A -0.50817
433A -> 439A 0.27180
434A -> 439A -0.10827
436A -> 442A -0.14246
436A -> 446A 0.14354
430B -> 440B -0.11132
431B -> 440B 0.18579
432B -> 439B 0.50817
433B -> 439B -0.27181
434B -> 439B 0.10828
436B -> 442B 0.14243
436B -> 446B -0.14353

Excited State 155: 3.000-A 2.7627 eV 448.79 nm f=0.0000 <S**2>=2.000
430A -> 439A 0.13326
431A -> 439A -0.22064
432A -> 440A -0.54554
433A -> 440A 0.29408
434A -> 440A -0.14580
430B -> 439B -0.13326
431B -> 439B 0.22064
432B -> 440B 0.54555
433B -> 440B -0.29409
434B -> 440B 0.14581

Excited State 156: 3.000-A 2.7671 eV 448.07 nm f=0.0000 <S**2>=2.000

398A -> 437A -0.14479
400A -> 438A 0.17995
401A -> 437A -0.32879
403A -> 437A 0.17906
405A -> 438A -0.29568
406A -> 437A -0.21446
407A -> 437A 0.10127
408A -> 438A 0.21684
409A -> 437A 0.11021
411A -> 438A 0.10276
435A -> 441A -0.18567
398B -> 437B 0.14692
400B -> 438B -0.18016
401B -> 437B 0.33022
403B -> 437B -0.18074
405B -> 438B 0.29574
406B -> 437B 0.21480
407B -> 437B -0.10215
408B -> 438B -0.21727
409B -> 437B -0.11019
411B -> 438B -0.10288
435B -> 441B 0.18587

Excited State 157: 1.000-A 2.7709 eV 447.46 nm f=0.0039 <S**2>=0.000
398A -> 437A 0.44310
399A -> 438A -0.22484
401A -> 437A 0.22016
402A -> 438A -0.10568
403A -> 437A -0.32769
407A -> 437A -0.18113
398B -> 437B 0.44226
399B -> 438B -0.22490
401B -> 437B 0.21851
402B -> 438B -0.10521
403B -> 437B -0.32679
407B -> 437B -0.18052

Excited State 158: 1.000-A 2.7728 eV 447.14 nm f=0.0203 <S**2>=0.000

| | |
|---|---|
| 398A -> 438A | -0.20938 |
| 399A -> 437A | 0.31697 |
| 400A -> 437A | -0.22978 |
| 401A -> 438A | 0.11815 |
| 402A -> 437A | -0.20322 |
| 403A -> 438A | 0.12166 |
| 404A -> 437A | -0.10870 |
| 405A -> 437A | 0.25166 |
| 406A -> 438A | 0.19155 |
| 409A -> 438A | -0.22841 |
| 410A -> 437A | -0.14968 |
| 398B -> 438B | -0.20896 |
| 399B -> 437B | 0.31695 |
| 400B -> 437B | -0.23013 |
| 401B -> 438B | 0.11884 |
| 402B -> 437B | -0.20416 |
| 403B -> 438B | 0.12124 |
| 404B -> 437B | -0.10870 |
| 405B -> 437B | 0.25201 |
| 406B -> 438B | 0.19190 |
| 409B -> 438B | -0.22859 |
| 410B -> 437B | -0.14983 |

Excited State 159: 3.000-A 2.7753 eV 446.74 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 398A -> 438A | -0.10097 |
| 401A -> 438A | -0.11646 |
| 402A -> 437A | 0.20241 |
| 405A -> 437A | -0.10093 |
| 433A -> 441A | 0.28865 |
| 435A -> 442A | -0.49871 |
| 398B -> 438B | 0.10151 |
| 401B -> 438B | 0.11638 |
| 402B -> 437B | -0.20215 |
| 405B -> 437B | 0.10045 |

433B -> 441B -0.28869
435B -> 442B 0.49879

Excited State 160: 1.000-A 2.7760 eV 446.64 nm f=0.0011 <S**2>=0.000
430A -> 440A -0.11007
431A -> 440A 0.21274
432A -> 439A 0.62152
433A -> 439A -0.19356
434A -> 439A 0.10406
430B -> 440B -0.11008
431B -> 440B 0.21275
432B -> 439B 0.62152
433B -> 439B -0.19357
434B -> 439B 0.10407

Excited State 161: 3.000-A 2.7774 eV 446.41 nm f=0.0000 <S**2>=2.000
401A -> 437A -0.15762
433A -> 442A -0.27551
435A -> 441A 0.53304
436A -> 441A 0.18991
401B -> 437B 0.15778
433B -> 442B 0.27552
435B -> 441B -0.53303
436B -> 441B -0.18997

Excited State 162: 3.000-A 2.7847 eV 445.23 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.16944
401A -> 438A 0.28103
402A -> 437A -0.38186
403A -> 438A -0.16010
405A -> 437A 0.17690
406A -> 438A 0.19111
410A -> 437A -0.10784
433A -> 441A 0.13300
435A -> 442A -0.23746
400B -> 437B 0.16917

401B -> 438B -0.28115
402B -> 437B 0.38199
403B -> 438B 0.16055
405B -> 437B -0.17661
406B -> 438B -0.19094
410B -> 437B 0.10767
433B -> 441B -0.13299
435B -> 442B 0.23736

Excited State 163: 1.000-A 2.7849 eV 445.20 nm f=0.0001 <S**2>=0.000
400A -> 438A 0.11897
401A -> 437A -0.21009
405A -> 438A -0.22150
408A -> 438A 0.17284
436A -> 441A 0.21798
436A -> 443A 0.50746
400B -> 438B 0.11872
401B -> 437B -0.20964
405B -> 438B -0.22115
408B -> 438B 0.17260
436B -> 441B 0.21787
436B -> 443B 0.50747

Excited State 164: 1.000-A 2.7850 eV 445.19 nm f=0.0000 <S**2>=0.000
430A -> 439A -0.11700
431A -> 439A 0.23138
432A -> 440A 0.60922
433A -> 440A -0.18292
434A -> 440A 0.11849
430B -> 439B -0.11700
431B -> 439B 0.23137
432B -> 440B 0.60921
433B -> 440B -0.18292
434B -> 440B 0.11849

Excited State 165: 1.000-A 2.7925 eV 443.99 nm f=0.0025 <S**2>=0.000

399A -> 438A 0.13777
400A -> 438A -0.14844
401A -> 437A 0.23071
405A -> 438A 0.29995
408A -> 438A -0.24561
409A -> 437A -0.13162
410A -> 438A -0.15513
411A -> 438A -0.12087
436A -> 441A 0.12208
436A -> 443A 0.38456
399B -> 438B 0.13770
400B -> 438B -0.14824
401B -> 437B 0.23040
405B -> 438B 0.29966
408B -> 438B -0.24543
409B -> 437B -0.13154
410B -> 438B -0.15507
411B -> 438B -0.12077
436B -> 441B 0.12220
436B -> 443B 0.38454

Excited State 166: 1.000-A 2.8086 eV 441.44 nm f=0.0433 <S**2>=0.000
398A -> 438A -0.26394
401A -> 438A -0.30434
402A -> 437A 0.40133
403A -> 438A 0.26021
406A -> 438A -0.10261
407A -> 438A -0.10560
409A -> 438A -0.11624
436A -> 442A -0.11972
398B -> 438B -0.26373
401B -> 438B -0.30394
402B -> 437B 0.40098
403B -> 438B 0.25996
406B -> 438B -0.10242
407B -> 438B -0.10561

409B -> 438B -0.11646
436B -> 442B -0.11973

Excited State 167: 1.000-A 2.8105 eV 441.14 nm f=0.0182 <S**2>=0.000
402A -> 437A 0.10763
436A -> 442A 0.49064
436A -> 444A 0.42732
436A -> 446A -0.12486
402B -> 437B 0.10762
436B -> 442B 0.49065
436B -> 444B 0.42732
436B -> 446B -0.12486

Excited State 168: 3.000-A 2.8218 eV 439.38 nm f=0.0000 <S**2>=2.000
431A -> 443A 0.14688
432A -> 446A -0.16271
434A -> 444A 0.23035
434A -> 446A 0.10862
436A -> 441A 0.34108
436A -> 443A 0.12968
436A -> 448A -0.34010
436A -> 463A 0.11552
431B -> 443B -0.14688
432B -> 446B 0.16271
434B -> 444B -0.23035
434B -> 446B -0.10862
436B -> 441B -0.34107
436B -> 443B -0.12969
436B -> 448B 0.34010
436B -> 463B -0.11552

Excited State 169: 3.000-A 2.8280 eV 438.42 nm f=0.0000 <S**2>=2.000
401A -> 438A 0.11953
402A -> 437A 0.24090
405A -> 437A -0.11173
406A -> 438A -0.10047

408A -> 437A -0.13524
409A -> 438A -0.52877
410A -> 437A -0.22101
412A -> 438A -0.13062
401B -> 438B -0.12054
402B -> 437B -0.24178
405B -> 437B 0.11234
406B -> 438B 0.10101
408B -> 437B 0.13612
409B -> 438B 0.53145
410B -> 437B 0.22213
412B -> 438B 0.13127

Excited State 170: 3.000-A 2.8319 eV 437.82 nm f=0.0000 <S**2>=2.000
402A -> 438A 0.18669
404A -> 438A -0.19624
405A -> 438A -0.11800
406A -> 437A -0.10703
408A -> 438A -0.10591
409A -> 437A -0.24659
410A -> 438A -0.40728
436A -> 441A 0.30890
402B -> 438B -0.18729
404B -> 438B 0.19699
405B -> 438B 0.11864
406B -> 437B 0.10743
408B -> 438B 0.10601
409B -> 437B 0.24727
410B -> 438B 0.40857
436B -> 441B -0.30924

Excited State 171: 1.000-A 2.8319 eV 437.81 nm f=0.0081 <S**2>=0.000
398A -> 438A -0.15632
401A -> 438A -0.16812
402A -> 437A -0.18106
403A -> 438A 0.15546

405A -> 437A 0.11871
406A -> 438A 0.11158
407A -> 438A -0.10055
408A -> 437A 0.15926
409A -> 438A 0.49343
410A -> 437A 0.21029
412A -> 438A 0.11964
398B -> 438B -0.15587
401B -> 438B -0.16745
402B -> 437B -0.17975
403B -> 438B 0.15492
405B -> 437B 0.11808
406B -> 438B 0.11099
407B -> 438B -0.10034
408B -> 437B 0.15850
409B -> 438B 0.49057
410B -> 437B 0.20905
412B -> 438B 0.11893

Excited State 172: 1.001-A 2.8374 eV 436.97 nm f=0.0020 <S**2>=0.000
400A -> 438A -0.10737
402A -> 438A -0.17978
404A -> 438A 0.21717
405A -> 438A 0.18329
406A -> 437A 0.12313
409A -> 437A 0.21136
410A -> 438A 0.38691
436A -> 441A -0.34219
436A -> 443A 0.16473
400B -> 438B -0.10872
402B -> 438B -0.18163
404B -> 438B 0.21967
405B -> 438B 0.18512
406B -> 437B 0.12479
409B -> 437B 0.21396
410B -> 438B 0.39161

436B -> 441B -0.33021
436B -> 443B 0.16096

Excited State 173: 3.000-A 2.8378 eV 436.90 nm f=0.0000 <S**2>=2.000
402A -> 438A 0.10361
404A -> 438A -0.13220
409A -> 437A -0.14370
410A -> 438A -0.25358
436A -> 441A -0.47952
436A -> 443A 0.15138
436A -> 448A -0.17362
404B -> 438B 0.12736
409B -> 437B 0.13897
410B -> 438B 0.24493
436B -> 441B 0.48808
436B -> 443B -0.15543
436B -> 448B 0.17384

Excited State 174: 1.000-A 2.8416 eV 436.32 nm f=0.0010 <S**2>=0.000
402A -> 438A -0.10963
404A -> 438A 0.13487
405A -> 438A 0.13091
409A -> 437A 0.13479
410A -> 438A 0.23417
436A -> 441A 0.55077
436A -> 443A -0.20532
402B -> 438B -0.10930
404B -> 438B 0.13451
405B -> 438B 0.13061
409B -> 437B 0.13433
410B -> 438B 0.23342
436B -> 441B 0.55040
436B -> 443B -0.20519

Excited State 175: 3.000-A 2.8788 eV 430.68 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.19638

402A -> 437A 0.26505
403A -> 438A -0.25663
406A -> 438A 0.10555
407A -> 438A -0.46734
408A -> 437A 0.18759
436A -> 442A 0.13466
400B -> 437B 0.19939
402B -> 437B -0.26816
403B -> 438B 0.26076
406B -> 438B -0.10741
407B -> 438B 0.47232
408B -> 437B -0.18947
436B -> 442B -0.13479

Excited State 176: 1.000-A 2.8808 eV 430.39 nm f=0.0004 <S**2>=0.000
400A -> 437A 0.25387
402A -> 437A -0.26353
403A -> 438A 0.34277
406A -> 438A -0.15445
407A -> 438A 0.41382
408A -> 437A -0.15840
400B -> 437B 0.25164
402B -> 437B -0.26048
403B -> 438B 0.33982
406B -> 438B -0.15345
407B -> 438B 0.40821
408B -> 437B -0.15610

Excited State 177: 3.000-A 2.8841 eV 429.89 nm f=0.0000 <S**2>=2.000
402A -> 438A -0.14822
403A -> 437A 0.10270
404A -> 438A 0.13666
405A -> 438A -0.24025
406A -> 437A 0.10606
407A -> 437A 0.26227
408A -> 438A -0.52968

402B -> 438B 0.14898
403B -> 437B -0.10302
404B -> 438B -0.13746
405B -> 438B 0.24223
406B -> 437B -0.10672
407B -> 437B -0.26382
408B -> 438B 0.53287

Excited State 178: 3.000-A 2.8846 eV 429.82 nm f=0.0000 <S**2>=2.000
407A -> 438A 0.13936
436A -> 442A 0.55975
436A -> 444A -0.18254
436A -> 446A 0.23923
407B -> 438B -0.13897
436B -> 442B -0.55972
436B -> 444B 0.18250
436B -> 446B -0.23922

Excited State 179: 1.000-A 2.8872 eV 429.43 nm f=0.0000 <S**2>=0.000
402A -> 438A 0.11869
404A -> 438A -0.13774
405A -> 438A 0.31691
406A -> 437A -0.11114
407A -> 437A -0.25584
408A -> 438A 0.51442
402B -> 438B 0.11775
404B -> 438B -0.13685
405B -> 438B 0.31545
406B -> 437B -0.11047
407B -> 437B -0.25418
408B -> 438B 0.51115

Excited State 180: 1.000-A 2.8890 eV 429.16 nm f=0.0068 <S**2>=0.000
400A -> 437A -0.13997
401A -> 438A -0.11538
402A -> 437A 0.10414

405A -> 437A -0.16306
406A -> 438A 0.46738
407A -> 438A 0.31832
408A -> 437A -0.17313
410A -> 437A 0.10778
436A -> 442A -0.10671
436A -> 444A 0.12745
400B -> 437B -0.14202
401B -> 438B -0.11689
402B -> 437B 0.10672
405B -> 437B -0.16529
406B -> 438B 0.47503
407B -> 438B 0.32182
408B -> 437B -0.17528
410B -> 437B 0.10967
436B -> 442B -0.10783
436B -> 444B 0.12783

Excited State 181: 3.000-A 2.8903 eV 428.97 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.13878
401A -> 438A -0.10378
402A -> 437A 0.17795
405A -> 437A -0.15494
406A -> 438A 0.53153
407A -> 438A 0.24841
408A -> 437A -0.15374
410A -> 437A 0.13205
400B -> 437B 0.13655
401B -> 438B 0.10218
402B -> 437B -0.17630
405B -> 437B 0.15257
406B -> 438B -0.52489
407B -> 438B -0.24415
408B -> 437B 0.15136
410B -> 437B -0.13050

Excited State 182: 1.000-A 2.8934 eV 428.51 nm f=0.0082 <S**2>=0.000

| | |
|---|---|
| 406A -> 438A | -0.16381 |
| 436A -> 442A | -0.44055 |
| 436A -> 444A | 0.49247 |
| 406B -> 438B | -0.16298 |
| 436B -> 442B | -0.44065 |
| 436B -> 444B | 0.49250 |

Excited State 183: 3.000-A 2.9072 eV 426.48 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 392A -> 439A | -0.34503 |
| 393A -> 440A | -0.36549 |
| 394A -> 439A | -0.10747 |
| 407A -> 440A | 0.10462 |
| 408A -> 439A | -0.10523 |
| 409A -> 440A | -0.10211 |
| 410A -> 439A | -0.11388 |
| 431A -> 439A | -0.18489 |
| 432A -> 440A | 0.18333 |
| 392B -> 439B | 0.34504 |
| 393B -> 440B | 0.36550 |
| 394B -> 439B | 0.10745 |
| 407B -> 440B | -0.10462 |
| 408B -> 439B | 0.10523 |
| 409B -> 440B | 0.10212 |
| 410B -> 439B | 0.11388 |
| 431B -> 439B | 0.18490 |
| 432B -> 440B | -0.18333 |

Excited State 184: 3.000-A 2.9074 eV 426.44 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 392A -> 440A | 0.36174 |
| 393A -> 439A | 0.38983 |
| 394A -> 440A | 0.11367 |
| 407A -> 439A | -0.11072 |
| 408A -> 440A | 0.11068 |
| 409A -> 439A | 0.10821 |
| 410A -> 440A | 0.11966 |

431A -> 440A 0.16159
432A -> 439A -0.16616
392B -> 440B -0.36176
393B -> 439B -0.38983
394B -> 440B -0.11366
407B -> 439B 0.11072
408B -> 440B -0.11068
409B -> 439B -0.10821
410B -> 440B -0.11966
431B -> 440B -0.16159
432B -> 439B 0.16616

Excited State 185: 3.000-A 2.9089 eV 426.23 nm f=0.0000 <S**2>=2.000
400A -> 438A 0.31721
401A -> 437A 0.16332
402A -> 438A -0.38894
403A -> 437A 0.25909
405A -> 438A 0.21701
406A -> 437A -0.16010
410A -> 438A -0.13158
411A -> 438A 0.13628
400B -> 438B -0.31804
401B -> 437B -0.16357
402B -> 438B 0.38982
403B -> 437B -0.25950
405B -> 438B -0.21736
406B -> 437B 0.16036
410B -> 438B 0.13182
411B -> 438B -0.13650

Excited State 186: 1.000-A 2.9187 eV 424.79 nm f=0.0001 <S**2>=0.000
400A -> 438A -0.39113
401A -> 437A -0.10636
402A -> 438A 0.43346
403A -> 437A -0.20525
405A -> 438A -0.17446

406A -> 437A 0.14041
410A -> 438A 0.11860
411A -> 438A -0.11437
400B -> 438B -0.39047
401B -> 437B -0.10604
402B -> 438B 0.43260
403B -> 437B -0.20469
405B -> 438B -0.17403
406B -> 437B 0.14005
410B -> 438B 0.11833
411B -> 438B -0.11407

Excited State 187: 1.000-A 2.9244 eV 423.96 nm f=0.0338 <S**2>=0.000
395A -> 437A -0.14179
396A -> 438A -0.16315
398A -> 438A 0.15555
400A -> 437A 0.31500
401A -> 438A 0.24493
402A -> 437A 0.20126
403A -> 438A 0.25224
404A -> 437A 0.10754
406A -> 438A 0.26019
407A -> 438A -0.11425
435A -> 442A 0.12257
395B -> 437B -0.14162
396B -> 438B -0.16313
398B -> 438B 0.15579
400B -> 437B 0.31587
401B -> 438B 0.24580
402B -> 437B 0.20158
403B -> 438B 0.25303
404B -> 437B 0.10779
406B -> 438B 0.26073
407B -> 438B -0.11453
435B -> 442B 0.12254

Excited State 188: 3.000-A 2.9336 eV 422.63 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 400A -> 437A | 0.35264 |
| 401A -> 438A | 0.35361 |
| 402A -> 437A | 0.15786 |
| 403A -> 438A | 0.32493 |
| 404A -> 437A | 0.10285 |
| 405A -> 437A | 0.13404 |
| 406A -> 438A | 0.22558 |
| 407A -> 438A | -0.11210 |
| 400B -> 437B | -0.35187 |
| 401B -> 438B | -0.35310 |
| 402B -> 437B | -0.15738 |
| 403B -> 438B | -0.32431 |
| 404B -> 437B | -0.10261 |
| 405B -> 437B | -0.13378 |
| 406B -> 438B | -0.22501 |
| 407B -> 438B | 0.11184 |

Excited State 189: 1.000-A 2.9389 eV 421.87 nm f=0.0000 <S**2>=0.000

| | |
|---|---|
| 430A -> 439A | 0.14241 |
| 431A -> 439A | 0.62540 |
| 432A -> 440A | -0.24465 |
| 434A -> 440A | 0.14963 |
| 430B -> 439B | 0.14272 |
| 431B -> 439B | 0.62670 |
| 432B -> 440B | -0.24510 |
| 434B -> 440B | 0.14995 |

Excited State 190: 3.000-A 2.9391 eV 421.84 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 392A -> 439A | -0.15085 |
| 393A -> 440A | -0.16084 |
| 430A -> 439A | 0.13906 |
| 431A -> 439A | 0.57936 |
| 432A -> 440A | -0.20345 |
| 434A -> 440A | 0.14143 |
| 392B -> 439B | 0.15085 |

393B -> 440B 0.16084
430B -> 439B -0.13874
431B -> 439B -0.57795
432B -> 440B 0.20290
434B -> 440B -0.14109

Excited State 191: 3.000-A 2.9429 eV 421.30 nm f=0.0000 <S**2>=2.000
400A -> 438A -0.36480
401A -> 437A -0.20941
402A -> 438A -0.40374
403A -> 437A -0.21657
404A -> 438A -0.15943
405A -> 438A -0.10180
406A -> 437A -0.13560
410A -> 438A -0.13377
411A -> 438A 0.11208
400B -> 438B 0.36601
401B -> 437B 0.20999
402B -> 438B 0.40502
403B -> 437B 0.21712
404B -> 438B 0.15999
405B -> 438B 0.10197
406B -> 437B 0.13599
410B -> 438B 0.13416
411B -> 438B -0.11236

Excited State 192: 1.000-A 2.9467 eV 420.76 nm f=0.0002 <S**2>=0.000
430A -> 440A 0.10891
431A -> 440A 0.64010
432A -> 439A -0.22856
434A -> 439A 0.14664
430B -> 440B 0.10893
431B -> 440B 0.64025
432B -> 439B -0.22861
434B -> 439B 0.14667

Excited State 193: 3.000-A 2.9479 eV 420.59 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 392A -> 440A | -0.12454 |
| 393A -> 439A | -0.13424 |
| 431A -> 440A | 0.60853 |
| 432A -> 439A | -0.21011 |
| 434A -> 439A | 0.14147 |
| 392B -> 440B | 0.12454 |
| 393B -> 439B | 0.13424 |
| 431B -> 440B | -0.60838 |
| 432B -> 439B | 0.21005 |
| 434B -> 439B | -0.14143 |

Excited State 194: 1.000-A 2.9496 eV 420.34 nm f=0.0004 <S**2>=0.000

| | |
|---|---|
| 400A -> 438A | 0.39087 |
| 401A -> 437A | 0.17179 |
| 402A -> 438A | 0.41565 |
| 403A -> 437A | 0.18590 |
| 404A -> 438A | 0.17521 |
| 406A -> 437A | 0.12705 |
| 410A -> 438A | 0.12668 |
| 400B -> 438B | 0.38976 |
| 401B -> 437B | 0.17114 |
| 402B -> 438B | 0.41443 |
| 403B -> 437B | 0.18522 |
| 404B -> 438B | 0.17473 |
| 406B -> 437B | 0.12663 |
| 410B -> 438B | 0.12628 |

Excited State 195: 1.000-A 2.9585 eV 419.08 nm f=0.0028 <S**2>=0.000

| | |
|---|---|
| 395A -> 438A | 0.26069 |
| 396A -> 437A | 0.35533 |
| 397A -> 437A | 0.28012 |
| 399A -> 438A | -0.11666 |
| 401A -> 437A | 0.20364 |
| 435A -> 441A | -0.34484 |
| 395B -> 438B | 0.26063 |

396B -> 437B 0.35532
397B -> 437B 0.28021
399B -> 438B -0.11674
401B -> 437B 0.20357
435B -> 441B -0.34485

Excited State 196: 1.000-A 2.9726 eV 417.08 nm f=0.0462 <S**2>=0.000
394A -> 437A -0.11611
395A -> 437A 0.27750
396A -> 438A 0.23528
397A -> 438A 0.16294
398A -> 438A -0.12005
399A -> 437A -0.13590
400A -> 437A 0.11812
401A -> 438A 0.34218
403A -> 438A 0.12364
435A -> 442A -0.33212
394B -> 437B -0.11615
395B -> 437B 0.27747
396B -> 438B 0.23527
397B -> 438B 0.16296
398B -> 438B -0.12016
399B -> 437B -0.13597
400B -> 437B 0.11803
401B -> 438B 0.34216
403B -> 438B 0.12355
435B -> 442B -0.33214

Excited State 197: 3.000-A 2.9892 eV 414.78 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.17177
430A -> 439A -0.64343
431A -> 439A 0.10916
432A -> 440A -0.18708
429B -> 439B 0.17181
430B -> 439B 0.64353
431B -> 439B -0.10917

| | | | | | |
|---|---|---|---|---|---|
| 432B -> 440B | 0.18711 | | | | |
| | | | | | |
| Excited State 198: | 3.000-A | 2.9900 eV | 414.66 nm | f=0.0000 | <S**2>=2.000 |
| 431A -> 444A | -0.17466 | | | | |
| 431A -> 446A | 0.10409 | | | | |
| 434A -> 443A | -0.43189 | | | | |
| 434A -> 448A | 0.14777 | | | | |
| 436A -> 444A | -0.38764 | | | | |
| 436A -> 446A | -0.16601 | | | | |
| 431B -> 444B | 0.17466 | | | | |
| 431B -> 446B | -0.10409 | | | | |
| 434B -> 443B | 0.43188 | | | | |
| 434B -> 448B | -0.14777 | | | | |
| 436B -> 444B | 0.38764 | | | | |
| 436B -> 446B | 0.16601 | | | | |
| | | | | | |
| Excited State 199: | 1.000-A | 2.9972 eV | 413.67 nm | f=0.0000 | <S**2>=0.000 |
| 429A -> 439A | 0.16234 | | | | |
| 430A -> 439A | 0.65766 | | | | |
| 431A -> 439A | -0.10097 | | | | |
| 432A -> 440A | 0.15303 | | | | |
| 429B -> 439B | 0.16232 | | | | |
| 430B -> 439B | 0.65755 | | | | |
| 431B -> 439B | -0.10096 | | | | |
| 432B -> 440B | 0.15301 | | | | |
| | | | | | |
| Excited State 200: | 3.000-A | 3.0058 eV | 412.48 nm | f=0.0000 | <S**2>=2.000 |
| 429A -> 440A | -0.16232 | | | | |
| 430A -> 440A | -0.66449 | | | | |
| 432A -> 439A | -0.15000 | | | | |
| 429B -> 440B | 0.16240 | | | | |
| 430B -> 440B | 0.66478 | | | | |
| 432B -> 439B | 0.15006 | | | | |

**Table S11.** Standard orientation of the optimized geometry for the open-ring isomer (OF4) of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | -0.18024 | -2.14154 | -0.21421 |
| N | -4.46048 | -2.55754 | 0.14895 |
| C | -3.41173 | -1.94397 | -0.51338 |
| C | -3.9597 | -1.22071 | -1.65747 |
| C | -5.36079 | -1.44221 | -1.66196 |
| C | -5.79125 | -2.34473 | -0.47736 |
| C | -6.74106 | -1.60105 | 0.436099 |
| C | -8.02737 | -1.95941 | 0.589833 |
| C | -8.588 | -3.16357 | -0.05481 |
| C | -7.65047 | -3.9928 | -0.83741 |
| C | -6.36323 | -3.64517 | -1.00486 |
| O | -9.79383 | -3.47519 | 0.072178 |
| C | -3.3761 | -0.46763 | -2.68178 |
| C | -4.20336 | 0.058606 | -3.68426 |
| C | -5.58839 | -0.1589 | -3.67762 |
| C | -6.17903 | -0.91927 | -2.65482 |
| C | -3.96517 | -3.40561 | 1.136753 |
| C | -2.58365 | -3.27231 | 1.05803 |
| N | -2.25309 | -2.34826 | 0.035624 |
| C | -4.83165 | -4.2572 | 1.979145 |
| C | -1.46792 | -3.96515 | 1.676591 |
| C | -1.59301 | -4.89171 | 2.72688 |
| C | -0.48035 | -5.61383 | 3.159835 |
| C | 0.753347 | -5.42082 | 2.52689 |
| C | 0.885903 | -4.47753 | 1.500448 |
| C | -0.20379 | -3.69481 | 1.075824 |
| C | -5.65377 | -3.69254 | 2.972049 |
| C | -6.48546 | -4.50437 | 3.74991 |
| C | -6.50106 | -5.8897 | 3.551965 |
| C | -5.67882 | -6.46251 | 2.573772 |
| C | -4.85159 | -5.65319 | 1.790518 |
| N | -4.00137 | 2.946959 | -0.16512 |
| C | -3.02761 | 2.216077 | 0.491191 |
| C | -3.65346 | 1.545001 | 1.627767 |
| C | -5.02099 | 1.92041 | 1.634309 |
| C | -5.34998 | 2.87072 | 0.455139 |
| C | -5.78684 | 4.220852 | 0.98633 |
| C | -7.03007 | 4.700543 | 0.813554 |
| C | -8.04385 | 3.976381 | 0.021098 |
| C | -7.60692 | 2.724084 | -0.62709 |
| C | -6.3655 | 2.233793 | -0.46841 |
| O | -9.2098 | 4.41254 | -0.11029 |
| C | -3.15858 | 0.71644 | 2.639935 |
| C | -4.03974 | 0.274479 | 3.636962 |
| C | -5.39077 | 0.648528 | 3.635821 |
| C | -5.89273 | 1.481418 | 2.622198 |
| C | -3.4189 | 3.737601 | -1.15262 |
| C | -2.06144 | 3.450498 | -1.07863 |
| N | -1.83325 | 2.494998 | -0.05882 |
| C | -4.18596 | 4.679142 | -1.99541 |
| C | -0.87801 | 3.993222 | -1.71747 |
| C | -0.8969 | 4.912293 | -2.78148 |
| C | 0.297138 | 5.452446 | -3.25996 |
| C | 1.51028 | 5.080454 | -2.66728 |
| C | 1.530739 | 4.148548 | -1.62348 |
| C | 0.350098 | 3.5598 | -1.14205 |
| C | -5.06547 | 4.207908 | -2.98796 |
| C | -5.80018 | 5.106876 | -3.76753 |
| C | -5.66044 | 6.485595 | -3.57183 |
| C | -4.7797 | 6.964553 | -2.59418 |
| C | -4.04893 | 6.06877 | -1.80906 |
| Cl | -0.23367 | 0.150683 | -1.64771 |
| Cl | -0.07315 | -0.1901 | 1.645214 |
| Ir | 0.199534 | 2.054527 | 0.196971 |
| N | 4.078316 | -2.50568 | -0.44468 |
| C | 2.980302 | -2.11671 | 0.300106 |
| C | 3.402731 | -1.93055 | 1.685458 |
| C | 4.78661 | -2.22455 | 1.741956 |
| C | 5.350333 | -2.54587 | 0.335962 |
| C | 5.972867 | -3.92338 | 0.300919 |
| C | 7.285289 | -4.12063 | 0.090191 |
| C | 8.20734 | -3.00445 | -0.20033 |
| C | 7.616381 | -1.65444 | -0.26242 |
| C | 6.305202 | -1.43542 | -0.05818 |
| O | 9.430346 | -3.19758 | -0.39113 |
| C | 2.70784 | -1.64486 | 2.865197 |
| C | 3.412547 | -1.64436 | 4.075935 |
| C | 4.783746 | -1.92858 | 4.121661 |
| C | 5.485258 | -2.2202 | 2.941743 |
| C | 3.65767 | -3.00433 | -1.68133 |
| C | 2.271775 | -2.86508 | -1.66809 |
| N | 1.873537 | -2.28671 | -0.44094 |
| C | 4.57849 | -3.6249 | -2.65358 |
| C | 1.178637 | -3.30738 | -2.52212 |
| C | 1.331228 | -3.82991 | -3.81791 |
| C | 0.224741 | -4.32827 | -4.50899 |
| C | -1.03565 | -4.31261 | -3.89988 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.19816 | -3.76552 | -2.62028 | H | -5.04183 | 4.760274 | 1.563791 |
| C | -0.11165 | -3.22122 | -1.91484 | H | -7.3401 | 5.649577 | 1.237064 |
| C | 5.651825 | -2.90308 | -3.20874 | H | -8.33753 | 2.231135 | -1.25935 |
| C | 6.540142 | -3.52179 | -4.094 | H | -6.04194 | 1.326758 | -0.96868 |
| C | 6.364552 | -4.8647 | -4.44635 | H | -2.12089 | 0.41288 | 2.641667 |
| C | 5.293774 | -5.58899 | -3.90773 | H | -3.65939 | -0.36483 | 4.426532 |
| C | 4.410166 | -4.97731 | -3.01495 | H | -6.0507 | 0.305942 | 4.42607 |
| N | 4.563354 | 1.764254 | 0.840705 | H | -6.93337 | 1.789856 | 2.621707 |
| C | 3.514047 | 1.671762 | -0.07168 | H | -1.83771 | 5.206048 | -3.23204 |
| C | 3.834066 | 1.430083 | -1.45388 | H | 0.281526 | 6.161074 | -4.08182 |
| C | 2.938454 | 0.777933 | -2.33135 | H | 2.442667 | 5.510233 | -3.02232 |
| C | 3.340139 | 0.362647 | -3.58919 | H | 2.479838 | 3.864618 | -1.1928 |
| C | 4.665149 | 0.586588 | -4.02625 | H | -5.16083 | 3.139772 | -3.15173 |
| C | 5.554088 | 1.264065 | -3.21046 | H | -6.47611 | 4.732127 | -4.52931 |
| C | 4.051867 | 2.234765 | 1.990602 | H | -6.23081 | 7.181602 | -4.17825 |
| C | 2.62114 | 2.383985 | 1.822468 | H | -4.66495 | 8.032671 | -2.44107 |
| N | 2.299158 | 1.953665 | 0.541675 | H | -3.36415 | 6.438371 | -1.05276 |
| C | 4.940065 | 2.517135 | 3.131332 | H | 5.297214 | -4.75038 | 0.498014 |
| C | 1.561981 | 2.951025 | 2.597745 | H | 7.722793 | -5.11289 | 0.103665 |
| C | 1.666899 | 3.391853 | 3.940089 | H | 8.299915 | -0.84143 | -0.48308 |
| C | 0.616779 | 4.078696 | 4.530635 | H | 5.879058 | -0.43625 | -0.0792 |
| C | -0.54994 | 4.349404 | 3.786322 | H | 1.652437 | -1.41957 | 2.838757 |
| C | -0.69014 | 3.872563 | 2.484024 | H | 2.879501 | -1.42341 | 4.994401 |
| C | 0.329979 | 3.114322 | 1.87092 | H | 5.30645 | -1.92764 | 5.072184 |
| C | 5.936577 | 1.584482 | 3.479209 | H | 6.544715 | -2.45365 | 2.968327 |
| C | 6.840813 | 1.85919 | 4.507153 | H | 2.30956 | -3.8518 | -4.28458 |
| C | 6.778288 | 3.076663 | 5.196405 | H | 0.346769 | -4.73134 | -5.50944 |
| C | 5.808487 | 4.021714 | 4.842845 | H | -1.89649 | -4.71788 | -4.42495 |
| C | 4.898194 | 3.747094 | 3.818223 | H | -2.18709 | -3.75203 | -2.17728 |
| H | -6.32787 | -0.72929 | 0.93335 | H | 5.78326 | -1.85876 | -2.95161 |
| H | -8.70756 | -1.39037 | 1.214485 | H | 7.366804 | -2.95471 | -4.50987 |
| H | -8.05436 | -4.90717 | -1.25803 | H | 7.055113 | -5.34258 | -5.13369 |
| H | -5.67434 | -4.26187 | -1.57455 | H | 5.151919 | -6.6312 | -4.17521 |
| H | -2.31052 | -0.28741 | -2.69191 | H | 3.585361 | -5.54124 | -2.5922 |
| H | -3.75358 | 0.636971 | -4.48439 | H | 1.940913 | 0.548621 | -1.99269 |
| H | -6.20676 | 0.246793 | -4.47154 | H | 2.635756 | -0.16383 | -4.22376 |
| H | -7.24755 | -1.10958 | -2.65113 | H | 4.976736 | 0.255418 | -5.01143 |
| H | -2.55518 | -5.05445 | 3.198656 | H | 6.542883 | 1.507743 | -3.58245 |
| H | -0.57763 | -6.32823 | 3.971163 | H | 2.563457 | 3.184048 | 4.509141 |
| H | 1.618504 | -6.00041 | 2.837295 | H | 0.695513 | 4.412941 | 5.559853 |
| H | 1.854959 | -4.35273 | 1.035008 | H | -1.35545 | 4.919681 | 4.240621 |
| H | -5.62912 | -2.62051 | 3.136676 | H | -1.60785 | 4.071426 | 1.944856 |
| H | -7.11608 | -4.05732 | 4.511643 | H | 5.989097 | 0.648363 | 2.93727 |
| H | -7.14651 | -6.51842 | 4.156668 | H | 7.598289 | 1.126365 | 4.767162 |
| H | -5.68466 | -7.5365 | 2.418609 | H | 7.485435 | 3.291727 | 5.991085 |
| H | -4.21151 | -6.09579 | 1.034374 | H | 5.770052 | 4.97922 | 5.352376 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 4.174606 | 4.500509 | 3.527689 | C | 6.3899 | 4.863791 | -0.15656 |
| C | 5.153828 | 1.772708 | -1.941 | H | 4.475463 | 4.09831 | -0.65162 |
| C | 6.033238 | 2.71129 | -1.27677 | H | 9.397056 | 3.302986 | -0.82841 |
| C | 7.462491 | 2.5441 | -1.35873 | H | 6.018846 | 5.789849 | 0.267493 |
| C | 5.543588 | 3.921068 | -0.66283 | C | 7.836991 | 4.681008 | -0.18006 |
| C | 8.323215 | 3.454189 | -0.81532 | O | 8.637209 | 5.538298 | 0.299855 |
| H | 7.851339 | 1.638741 | -1.81348 | | | | |

Excited State 1: 3.000-A -0.5916 eV -2095.64 nm f=-0.0000 <S**2>=2.000

433A -> 438A 0.18495

434A -> 438A -0.26904

435A -> 438A 0.50711

436A -> 438A 0.35183

433B -> 438B -0.18495

434B -> 438B 0.26904

435B -> 438B -0.50711

436B -> 438B -0.35183

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -6023.98914385

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.000-A -0.5811 eV -2133.57 nm f=-0.0000 <S**2>=2.000

433A -> 437A -0.23588

434A -> 437A -0.23222

435A -> 437A -0.36290

436A -> 437A 0.49689

433B -> 437B 0.23588

434B -> 437B 0.23222

435B -> 437B 0.36290

436B -> 437B -0.49689

Excited State 3: 3.000-A 0.5761 eV 2152.23 nm f=0.0000 <S**2>=2.000

431A -> 437A 0.15657

433A -> 437A 0.24932

434A -> 437A 0.37115

435A -> 437A 0.19870

436A -> 437A 0.47565

431B -> 437B -0.15657
433B -> 437B -0.24932
434B -> 437B -0.37115
435B -> 437B -0.19870
436B -> 437B -0.47565

Excited State 4: 1.000-A 0.6670 eV 1858.83 nm f=0.0073 <S**2>=0.000
434A -> 437A 0.11164
435A -> 437A 0.46884
436A -> 437A 0.51653
434B -> 437B 0.11164
435B -> 437B 0.46884
436B -> 437B 0.51653

Excited State 5: 3.000-A 0.6754 eV 1835.62 nm f=0.0000 <S**2>=2.000
430A -> 438A 0.14579
433A -> 438A -0.20647
434A -> 438A 0.32327
435A -> 438A -0.11830
436A -> 438A 0.55845
430B -> 438B -0.14579
433B -> 438B 0.20647
434B -> 438B -0.32327
435B -> 438B 0.11830
436B -> 438B -0.55845

Excited State 6: 1.000-A 0.7020 eV 1766.03 nm f=0.0055 <S**2>=0.000
435A -> 438A -0.30309
436A -> 438A 0.62842
435B -> 438B -0.30309
436B -> 438B 0.62842

Excited State 7: 3.000-A 0.7216 eV 1718.26 nm f=0.0000 <S**2>=2.000
431A -> 437A -0.10962
433A -> 437A -0.28415
433A -> 438A 0.11327

434A -> 437A -0.21693
435A -> 437A 0.53689
435A -> 438A -0.16693
436A -> 437A 0.13781
431B -> 437B 0.10962
433B -> 437B 0.28415
433B -> 438B -0.11327
434B -> 437B 0.21693
435B -> 437B -0.53689
435B -> 438B 0.16693
436B -> 437B -0.13781

Excited State 8: 3.000-A 0.7380 eV 1680.11 nm f=0.0000 <S**2>=2.000
430A -> 438A 0.14283
433A -> 437A -0.11098
433A -> 438A -0.32081
434A -> 438A 0.28442
435A -> 437A 0.18515
435A -> 438A 0.43677
436A -> 438A -0.22793
430B -> 438B -0.14283
433B -> 437B 0.11098
433B -> 438B 0.32081
434B -> 438B -0.28442
435B -> 437B -0.18515
435B -> 438B -0.43677
436B -> 438B 0.22793

Excited State 9: 1.000-A 0.8232 eV 1506.11 nm f=0.0422 <S**2>=0.000
433A -> 437A -0.30152
434A -> 437A -0.22337
435A -> 437A 0.46317
436A -> 437A -0.38849
433B -> 437B -0.30152
434B -> 437B -0.22337
435B -> 437B 0.46317

436B -> 437B -0.38849
436A <- 437A 0.12869
436B <- 437B 0.12869

Excited State 10: 1.000-A 0.9030 eV 1373.10 nm f=0.0912 <S**2>=0.000
433A -> 438A -0.28280
434A -> 438A 0.30879
435A -> 438A 0.51797
436A -> 438A 0.22676
433B -> 438B -0.28280
434B -> 438B 0.30879
435B -> 438B 0.51797
436B -> 438B 0.22676
435A <- 438A -0.10373
435B <- 438B -0.10373

Excited State 11: 3.000-A 0.9732 eV 1274.00 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.27441
432A -> 437A 0.54354
433A -> 437A 0.29490
434A -> 437A -0.11639
429B -> 437B -0.27441
432B -> 437B -0.54354
433B -> 437B -0.29490
434B -> 437B 0.11639

Excited State 12: 3.000-A 1.0457 eV 1185.70 nm f=0.0000 <S**2>=2.000
429A -> 438A -0.30834
430A -> 438A 0.13960
432A -> 438A 0.50757
433A -> 438A 0.28427
434A -> 438A 0.15747
429B -> 438B 0.30834
430B -> 438B -0.13960
432B -> 438B -0.50757
433B -> 438B -0.28427

434B -> 438B -0.15747

Excited State 13: 1.000-A 1.0587 eV 1171.11 nm f=0.0043 <S**2>=0.000
429A -> 437A 0.10488
432A -> 437A 0.26909
433A -> 437A 0.48886
434A -> 437A -0.39238
435A -> 437A 0.12888
429B -> 437B 0.10488
432B -> 437B 0.26909
433B -> 437B 0.48886
434B -> 437B -0.39238
435B -> 437B 0.12888

Excited State 14: 3.000-A 1.0806 eV 1147.32 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.11459
430A -> 437A -0.12271
432A -> 437A 0.25702
433A -> 437A -0.42210
434A -> 437A 0.46264
429B -> 437B -0.11459
430B -> 437B 0.12271
432B -> 437B -0.25702
433B -> 437B 0.42210
434B -> 437B -0.46264

Excited State 15: 1.000-A 1.0893 eV 1138.16 nm f=0.0253 <S**2>=0.000
429A -> 437A 0.17533
430A -> 437A -0.10012
432A -> 437A 0.45320
434A -> 437A 0.43870
435A -> 437A 0.10823
436A -> 437A -0.21193
429B -> 437B 0.17533
430B -> 437B -0.10012
432B -> 437B 0.45320

434B -> 437B 0.43870
435B -> 437B 0.10823
436B -> 437B -0.21193

Excited State 16: 1.000-A 1.1123 eV 1114.64 nm f=0.0020 <S**2>=0.000
429A -> 438A -0.10435
432A -> 438A 0.27714
433A -> 438A 0.51434
434A -> 438A 0.33783
435A -> 438A 0.13845
429B -> 438B -0.10435
432B -> 438B 0.27714
433B -> 438B 0.51434
434B -> 438B 0.33783
435B -> 438B 0.13845

Excited State 17: 3.000-A 1.1458 eV 1082.09 nm f=0.0000 <S**2>=2.000
423A -> 437A -0.11548
426A -> 438A -0.12219
429A -> 438A 0.16181
430A -> 438A -0.13038
431A -> 438A -0.10976
432A -> 438A -0.22017
433A -> 438A 0.42215
434A -> 438A 0.42059
423B -> 437B 0.11548
426B -> 438B 0.12219
429B -> 438B -0.16181
430B -> 438B 0.13038
431B -> 438B 0.10976
432B -> 438B 0.22017
433B -> 438B -0.42215
434B -> 438B -0.42059

Excited State 18: 3.000-A 1.1459 eV 1081.95 nm f=0.0000 <S**2>=2.000
423A -> 437A 0.68047

423B -> 437B -0.68047

Excited State 19: 3.000-A 1.1784 eV 1052.14 nm f=0.0000 <S**2>=2.000
425A -> 438A -0.23456
426A -> 438A 0.63316
425B -> 438B 0.23456
426B -> 438B -0.63316

Excited State 20: 1.000-A 1.2092 eV 1025.30 nm f=0.0355 <S**2>=0.000
429A -> 438A -0.20377
431A -> 438A 0.10349
432A -> 438A 0.52170
433A -> 438A -0.16430
434A -> 438A -0.30859
435A -> 438A 0.16179
436A -> 438A 0.13319
429B -> 438B -0.20377
431B -> 438B 0.10349
432B -> 438B 0.52170
433B -> 438B -0.16430
434B -> 438B -0.30859
435B -> 438B 0.16179
436B -> 438B 0.13319

Excited State 21: 3.000-A 1.2761 eV 971.60 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.10717
431A -> 437A 0.64964
433A -> 437A -0.12132
434A -> 437A -0.16669
429B -> 437B -0.10717
431B -> 437B -0.64964
433B -> 437B 0.12132
434B -> 437B 0.16669

Excited State 22: 1.000-A 1.3036 eV 951.08 nm f=0.0512 <S**2>=0.000
431A -> 437A 0.41978

432A -> 437A 0.31684
433A -> 437A -0.33298
434A -> 437A -0.22383
435A -> 437A -0.15088
436A -> 437A 0.17497
431B -> 437B 0.41978
432B -> 437B 0.31684
433B -> 437B -0.33298
434B -> 437B -0.22383
435B -> 437B -0.15088
436B -> 437B 0.17497
436A <- 437A -0.10297
436B <- 437B -0.10297

Excited State 23: 3.000-A 1.3213 eV 938.36 nm f=0.0000 <S**2>=2.000
427A -> 438A -0.17581
428A -> 438A 0.38461
429A -> 438A -0.28217
430A -> 438A -0.35125
431A -> 438A 0.25681
432A -> 438A -0.14652
427B -> 438B 0.17581
428B -> 438B -0.38461
429B -> 438B 0.28217
430B -> 438B 0.35125
431B -> 438B -0.25681
432B -> 438B 0.14652

Excited State 24: 1.000-A 1.3611 eV 910.93 nm f=0.1084 <S**2>=0.000
426A -> 438A -0.11995
430A -> 438A -0.20231
432A -> 438A 0.26487
433A -> 438A -0.32067
434A -> 438A 0.38408
435A -> 438A -0.30790
436A -> 438A -0.17853

426B -> 438B -0.11995
430B -> 438B -0.20231
432B -> 438B 0.26487
433B -> 438B -0.32067
434B -> 438B 0.38408
435B -> 438B -0.30790
436B -> 438B -0.17853
435A <- 438A 0.14118
435B <- 438B 0.14118

Excited State 25: 3.000-A 1.3717 eV 903.84 nm f=0.0000 <S**2>=2.000
428A -> 438A 0.23490
429A -> 438A -0.12674
430A -> 438A 0.51611
432A -> 438A -0.32834
433A -> 438A 0.15810
428B -> 438B -0.23490
429B -> 438B 0.12674
430B -> 438B -0.51611
432B -> 438B 0.32834
433B -> 438B -0.15810

Excited State 26: 1.000-A 1.3791 eV 899.03 nm f=0.0161 <S**2>=0.000
428A -> 437A 0.18383
429A -> 437A 0.19814
430A -> 437A -0.32874
431A -> 437A 0.42810
432A -> 437A -0.27921
433A -> 437A 0.14478
436A -> 437A -0.10017
428B -> 437B 0.18383
429B -> 437B 0.19814
430B -> 437B -0.32874
431B -> 437B 0.42810
432B -> 437B -0.27921
433B -> 437B 0.14478

436B -> 437B -0.10017

Excited State 27: 3.000-A 1.3800 eV 898.43 nm f=0.0000 <S**2>=2.000
427A -> 437A -0.16750
428A -> 437A -0.32786
429A -> 437A -0.23707
430A -> 437A 0.45339
431A -> 437A 0.11903
432A -> 437A 0.26841
427B -> 437B 0.16750
428B -> 437B 0.32786
429B -> 437B 0.23707
430B -> 437B -0.45339
431B -> 437B -0.11903
432B -> 437B -0.26841

Excited State 28: 1.000-A 1.4018 eV 884.47 nm f=0.0014 <S**2>=0.000
427A -> 438A -0.12130
428A -> 438A 0.38470
429A -> 438A -0.31932
430A -> 438A -0.20396
431A -> 438A 0.39989
432A -> 438A -0.15041
427B -> 438B -0.12130
428B -> 438B 0.38470
429B -> 438B -0.31932
430B -> 438B -0.20396
431B -> 438B 0.39989
432B -> 438B -0.15041

Excited State 29: 1.000-A 1.4515 eV 854.17 nm f=0.0393 <S**2>=0.000
423A -> 437A -0.13324
428A -> 437A -0.15484
429A -> 437A 0.13490
430A -> 437A 0.53795
431A -> 437A 0.24308

432A -> 437A -0.15169
433A -> 437A 0.10049
434A -> 437A 0.15708
436A -> 437A -0.13705
423B -> 437B -0.13324
428B -> 437B -0.15484
429B -> 437B 0.13490
430B -> 437B 0.53795
431B -> 437B 0.24308
432B -> 437B -0.15169
433B -> 437B 0.10049
434B -> 437B 0.15708
436B -> 437B -0.13705

Excited State 30: 3.000-A 1.4523 eV 853.70 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.54793
430A -> 437A 0.35679
432A -> 437A -0.21099
429B -> 437B -0.54793
430B -> 437B -0.35679
432B -> 437B 0.21099

Excited State 31: 3.000-A 1.4736 eV 841.34 nm f=0.0000 <S**2>=2.000
427A -> 437A 0.28018
428A -> 437A 0.49446
429A -> 437A -0.15369
430A -> 437A 0.37475
427B -> 437B -0.28018
428B -> 437B -0.49446
429B -> 437B 0.15369
430B -> 437B -0.37475

Excited State 32: 1.000-A 1.4741 eV 841.06 nm f=0.0169 <S**2>=0.000
426A -> 438A -0.21077
429A -> 437A 0.12896
429A -> 438A -0.23287

430A -> 438A 0.55710
431A -> 438A 0.11335
432A -> 438A -0.10809
434A -> 438A 0.13248
426B -> 438B -0.21077
429B -> 437B 0.12896
429B -> 438B -0.23287
430B -> 438B 0.55710
431B -> 438B 0.11335
432B -> 438B -0.10809
434B -> 438B 0.13248

Excited State 33: 1.000-A 1.4797 eV 837.90 nm f=0.0171 <S**2>=0.000
423A -> 437A 0.15849
429A -> 437A 0.59629
430A -> 438A -0.13379
431A -> 437A -0.21648
433A -> 437A -0.13365
423B -> 437B 0.15849
429B -> 437B 0.59629
430B -> 438B -0.13379
431B -> 437B -0.21648
433B -> 437B -0.13365

Excited State 34: 3.000-A 1.4989 eV 827.19 nm f=0.0000 <S**2>=2.000
429A -> 438A 0.41157
431A -> 438A 0.54277
432A -> 438A 0.13452
429B -> 438B -0.41157
431B -> 438B -0.54277
432B -> 438B -0.13452

Excited State 35: 1.000-A 1.5074 eV 822.50 nm f=0.0001 <S**2>=0.000
427A -> 437A 0.22088
428A -> 437A 0.52102
429A -> 438A -0.18350

430A -> 437A 0.22047
431A -> 438A -0.25037
427B -> 437B 0.22088
428B -> 437B 0.52102
429B -> 438B -0.18350
430B -> 437B 0.22047
431B -> 438B -0.25037

Excited State 36: 3.000-A 1.5084 eV 821.96 nm f=0.0000 <S**2>=2.000
427A -> 438A -0.11501
428A -> 438A 0.48506
429A -> 438A 0.30218
431A -> 438A -0.33216
432A -> 438A 0.18663
427B -> 438B 0.11501
428B -> 438B -0.48506
429B -> 438B -0.30218
431B -> 438B 0.33216
432B -> 438B -0.18663

Excited State 37: 1.000-A 1.5114 eV 820.31 nm f=0.0048 <S**2>=0.000
426A -> 438A 0.11428
427A -> 437A 0.12438
428A -> 437A 0.27241
428A -> 438A -0.17640
429A -> 438A 0.31888
430A -> 437A 0.14255
431A -> 438A 0.47306
426B -> 438B 0.11428
427B -> 437B 0.12438
428B -> 437B 0.27241
428B -> 438B -0.17640
429B -> 438B 0.31888
430B -> 437B 0.14255
431B -> 438B 0.47306

Excited State 38: 1.000-A 1.5261 eV 812.43 nm f=0.0108 <S**2>=0.000

| | |
|---|---|
| 423A -> 437A | 0.64907 |
| 431A -> 437A | 0.10930 |
| 423B -> 437B | 0.64907 |
| 431B -> 437B | 0.10930 |

Excited State 39: 1.000-A 1.5278 eV 811.54 nm f=0.0083 <S**2>=0.000

| | |
|---|---|
| 423A -> 437A | 0.12357 |
| 425A -> 438A | -0.13284 |
| 426A -> 438A | 0.42339 |
| 427A -> 438A | 0.10371 |
| 428A -> 438A | -0.35522 |
| 429A -> 438A | -0.33383 |
| 432A -> 438A | -0.10661 |
| 423B -> 437B | 0.12357 |
| 425B -> 438B | -0.13284 |
| 426B -> 438B | 0.42339 |
| 427B -> 438B | 0.10371 |
| 428B -> 438B | -0.35522 |
| 429B -> 438B | -0.33383 |
| 432B -> 438B | -0.10661 |

Excited State 40: 1.000-A 1.5541 eV 797.81 nm f=0.0169 <S**2>=0.000

| | |
|---|---|
| 425A -> 438A | -0.16494 |
| 426A -> 438A | 0.40172 |
| 428A -> 438A | 0.38976 |
| 429A -> 438A | 0.17072 |
| 430A -> 438A | 0.24906 |
| 431A -> 438A | -0.15862 |
| 432A -> 438A | 0.10291 |
| 435A -> 438A | -0.10302 |
| 425B -> 438B | -0.16494 |
| 426B -> 438B | 0.40172 |
| 428B -> 438B | 0.38976 |
| 429B -> 438B | 0.17072 |
| 430B -> 438B | 0.24906 |

431B -> 438B -0.15862
432B -> 438B 0.10291
435B -> 438B -0.10302

Excited State 41: 3.000-A 1.7057 eV 726.88 nm f=0.0000 <S**2>=2.000
427A -> 437A 0.59391
428A -> 437A -0.35275
427B -> 437B -0.59391
428B -> 437B 0.35275

Excited State 42: 1.000-A 1.7277 eV 717.65 nm f=0.0011 <S**2>=0.000
427A -> 437A 0.63286
428A -> 437A -0.28531
427B -> 437B 0.63286
428B -> 437B -0.28531

Excited State 43: 3.000-A 1.7857 eV 694.30 nm f=0.0000 <S**2>=2.000
422A -> 438A 0.13491
424A -> 438A -0.10605
425A -> 438A -0.13932
427A -> 438A 0.60205
428A -> 438A 0.18936
422B -> 438B -0.13491
424B -> 438B 0.10605
425B -> 438B 0.13932
427B -> 438B -0.60205
428B -> 438B -0.18936

Excited State 44: 3.000-A 1.8092 eV 685.29 nm f=0.0000 <S**2>=2.000
420A -> 437A -0.10108
421A -> 437A 0.10045
424A -> 437A -0.44497
425A -> 437A 0.46503
426A -> 437A 0.17792
420B -> 437B 0.10108
421B -> 437B -0.10045

424B -> 437B 0.44497
425B -> 437B -0.46503
426B -> 437B -0.17792

Excited State 45: 1.000-A 1.8384 eV 674.41 nm f=0.0123 <S**2>=0.000
427A -> 438A 0.67559
428A -> 438A 0.17095
427B -> 438B 0.67559
428B -> 438B 0.17095

Excited State 46: 3.000-A 1.9016 eV 652.00 nm f=0.0000 <S**2>=2.000
424A -> 438A 0.33840
425A -> 438A 0.51077
426A -> 438A 0.18665
427A -> 438A 0.20570
424B -> 438B -0.33840
425B -> 438B -0.51077
426B -> 438B -0.18665
427B -> 438B -0.20570

Excited State 47: 3.000-A 1.9042 eV 651.10 nm f=0.0000 <S**2>=2.000
402A -> 437A 0.18995
403A -> 437A 0.15970
404A -> 437A 0.11685
409A -> 437A 0.11868
413A -> 437A -0.17144
416A -> 437A 0.19348
417A -> 437A 0.19098
418A -> 437A -0.15977
419A -> 437A -0.10759
420A -> 437A 0.28552
421A -> 437A -0.18508
422A -> 437A 0.14916
425A -> 437A 0.15204
402B -> 437B -0.18995
403B -> 437B -0.15970

404B -> 437B -0.11685
409B -> 437B -0.11868
413B -> 437B 0.17144
416B -> 437B -0.19348
417B -> 437B -0.19098
418B -> 437B 0.15977
419B -> 437B 0.10759
420B -> 437B -0.28552
421B -> 437B 0.18508
422B -> 437B -0.14916
425B -> 437B -0.15204

Excited State 48: 3.000-A 1.9240 eV 644.41 nm f=0.0000 <S**2>=2.000
399A -> 438A -0.11776
404A -> 438A -0.10992
405A -> 438A 0.11120
406A -> 438A -0.10484
410A -> 438A -0.16631
416A -> 438A -0.12635
417A -> 438A 0.10313
418A -> 438A -0.13983
419A -> 438A 0.19982
420A -> 438A 0.23182
421A -> 438A 0.35060
422A -> 438A -0.17566
425A -> 438A -0.14132
427A -> 438A 0.15617
399B -> 438B 0.11776
404B -> 438B 0.10992
405B -> 438B -0.11120
406B -> 438B 0.10484
410B -> 438B 0.16631
416B -> 438B 0.12635
417B -> 438B -0.10313
418B -> 438B 0.13983
419B -> 438B -0.19982

420B -> 438B -0.23182
421B -> 438B -0.35060
422B -> 438B 0.17566
425B -> 438B 0.14132
427B -> 438B -0.15617

Excited State 49: 1.000-A 1.9345 eV 640.91 nm f=0.0157 <S**2>=0.000
424A -> 437A -0.44096
425A -> 437A 0.50374
426A -> 437A 0.19811
424B -> 437B -0.44096
425B -> 437B 0.50374
426B -> 437B 0.19811

Excited State 50: 1.000-A 1.9893 eV 623.25 nm f=0.0095 <S**2>=0.000
424A -> 438A 0.38671
425A -> 438A 0.53956
426A -> 438A 0.19845
424B -> 438B 0.38671
425B -> 438B 0.53956
426B -> 438B 0.19845

Excited State 51: 3.000-A 2.0284 eV 611.23 nm f=0.0000 <S**2>=2.000
422A -> 437A 0.22920
424A -> 437A 0.50590
425A -> 437A 0.37108
426A -> 437A 0.15042
422B -> 437B -0.22920
424B -> 437B -0.50590
425B -> 437B -0.37108
426B -> 437B -0.15042

Excited State 52: 1.000-A 2.0376 eV 608.47 nm f=0.0006 <S**2>=0.000
422A -> 437A 0.22100
424A -> 437A 0.51962
425A -> 437A 0.37314

426A -> 437A 0.15250
422B -> 437B 0.22100
424B -> 437B 0.51962
425B -> 437B 0.37314
426B -> 437B 0.15250

Excited State 53: 3.000-A 2.0479 eV 605.41 nm f=0.0000 <S**2>=2.000
409A -> 438A 0.13220
410A -> 438A 0.14324
411A -> 438A 0.22704
413A -> 438A -0.13772
415A -> 438A 0.12178
416A -> 438A -0.11976
419A -> 438A -0.13385
421A -> 438A 0.16320
422A -> 438A 0.30236
424A -> 438A 0.36337
425A -> 438A -0.12613
409B -> 438B -0.13220
410B -> 438B -0.14324
411B -> 438B -0.22704
413B -> 438B 0.13772
415B -> 438B -0.12178
416B -> 438B 0.11976
419B -> 438B 0.13385
421B -> 438B -0.16320
422B -> 438B -0.30236
424B -> 438B -0.36337
425B -> 438B 0.12613

Excited State 54: 3.000-A 2.0973 eV 591.16 nm f=0.0000 <S**2>=2.000
408A -> 438A -0.10015
410A -> 438A -0.20505
411A -> 438A -0.11756
413A -> 438A 0.10787
414A -> 438A 0.11315

415A -> 438A -0.15530
416A -> 438A 0.11622
418A -> 438A -0.12442
419A -> 438A 0.16073
420A -> 438A -0.20664
421A -> 438A -0.12839
422A -> 438A 0.13455
424A -> 438A 0.38642
425A -> 438A -0.20507
408B -> 438B 0.10015
410B -> 438B 0.20505
411B -> 438B 0.11756
413B -> 438B -0.10787
414B -> 438B -0.11315
415B -> 438B 0.15530
416B -> 438B -0.11622
418B -> 438B 0.12442
419B -> 438B -0.16073
420B -> 438B 0.20664
421B -> 438B 0.12839
422B -> 438B -0.13455
424B -> 438B -0.38642
425B -> 438B 0.20507

Excited State 55: 1.000-A 2.1004 eV 590.28 nm f=0.0015 <S**2>=0.000
422A -> 438A 0.27202
424A -> 438A 0.52982
425A -> 438A -0.33808
426A -> 438A -0.11900
422B -> 438B 0.27202
424B -> 438B 0.52982
425B -> 438B -0.33808
426B -> 438B -0.11900

Excited State 56: 3.000-A 2.1066 eV 588.54 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.14312

402A -> 437A 0.15079
403A -> 437A -0.22036
404A -> 437A 0.11141
407A -> 437A -0.15788
409A -> 437A -0.14678
413A -> 437A 0.24021
414A -> 437A -0.13422
415A -> 437A 0.15230
416A -> 437A -0.20940
417A -> 437A -0.15420
418A -> 437A -0.19832
420A -> 437A 0.10526
421A -> 437A -0.13258
422A -> 437A 0.22264
424A -> 437A -0.11616
400B -> 437B -0.14312
402B -> 437B -0.15079
403B -> 437B 0.22036
404B -> 437B -0.11141
407B -> 437B 0.15788
409B -> 437B 0.14678
413B -> 437B -0.24021
414B -> 437B 0.13422
415B -> 437B -0.15230
416B -> 437B 0.20940
417B -> 437B 0.15420
418B -> 437B 0.19832
420B -> 437B -0.10526
421B -> 437B 0.13258
422B -> 437B -0.22264
424B -> 437B 0.11616

Excited State 57: 3.000-A 2.1647 eV 572.75 nm f=0.0000 <S**2>=2.000
422A -> 437A -0.19334
425A -> 437A -0.17852
426A -> 437A 0.63921

422B -> 437B 0.19334
425B -> 437B 0.17852
426B -> 437B -0.63921

Excited State 58: 1.000-A 2.1655 eV 572.54 nm f=0.0001 <S**2>=0.000
422A -> 437A -0.11764
425A -> 437A -0.23435
426A -> 437A 0.65256
422B -> 437B -0.11764
425B -> 437B -0.23435
426B -> 437B 0.65256

Excited State 59: 3.000-A 2.1731 eV 570.54 nm f=0.0000 <S**2>=2.000
411A -> 438A -0.16303
413A -> 438A 0.17153
415A -> 438A -0.15862
416A -> 438A 0.14787
419A -> 438A -0.29504
421A -> 438A 0.30035
422A -> 438A -0.27609
424A -> 438A 0.16456
425A -> 438A -0.16417
411B -> 438B 0.16303
413B -> 438B -0.17153
415B -> 438B 0.15862
416B -> 438B -0.14787
419B -> 438B 0.29504
421B -> 438B -0.30035
422B -> 438B 0.27609
424B -> 438B -0.16456
425B -> 438B 0.16417

Excited State 60: 3.000-A 2.1751 eV 570.01 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.10195
402A -> 437A -0.16221
403A -> 437A 0.11497

404A -> 437A -0.12024
407A -> 437A 0.14808
412A -> 437A 0.13304
417A -> 437A 0.12047
422A -> 437A 0.49429
425A -> 437A -0.22926
426A -> 437A 0.17066
400B -> 437B 0.10195
402B -> 437B 0.16221
403B -> 437B -0.11497
404B -> 437B 0.12024
407B -> 437B -0.14808
412B -> 437B -0.13304
417B -> 437B -0.12047
422B -> 437B -0.49429
425B -> 437B 0.22926
426B -> 437B -0.17066

Excited State 61: 1.000-A 2.1880 eV 566.64 nm f=0.0025 <S**2>=0.000
420A -> 437A 0.18563
422A -> 437A 0.62184
424A -> 437A -0.14787
425A -> 437A -0.16653
420B -> 437B 0.18563
422B -> 437B 0.62184
424B -> 437B -0.14787
425B -> 437B -0.16653

Excited State 62: 3.000-A 2.1885 eV 566.53 nm f=0.0000 <S**2>=2.000
433A -> 439A 0.12064
436A -> 439A 0.68505
433B -> 439B -0.12064
436B -> 439B -0.68505

Excited State 63: 1.000-A 2.1937 eV 565.18 nm f=0.0002 <S**2>=0.000
433A -> 439A 0.11442

436A -> 439A 0.69037
433B -> 439B 0.11442
436B -> 439B 0.69037

Excited State 64: 3.000-A 2.2120 eV 560.50 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.10031
401A -> 437A 0.10381
402A -> 437A 0.20805
404A -> 437A 0.14066
412A -> 437A -0.15089
413A -> 437A -0.12756
417A -> 437A -0.17736
420A -> 437A -0.24063
421A -> 437A 0.38045
422A -> 437A 0.20846
425A -> 437A -0.14065
400B -> 437B -0.10031
401B -> 437B -0.10381
402B -> 437B -0.20805
404B -> 437B -0.14066
412B -> 437B 0.15089
413B -> 437B 0.12756
417B -> 437B 0.17736
420B -> 437B 0.24063
421B -> 437B -0.38045
422B -> 437B -0.20846
425B -> 437B 0.14065

Excited State 65: 1.000-A 2.2159 eV 559.53 nm f=0.0244 <S**2>=0.000
420A -> 438A -0.14579
421A -> 438A -0.25797
422A -> 438A 0.58338
424A -> 438A -0.18819
425A -> 438A 0.11740
420B -> 438B -0.14579
421B -> 438B -0.25797

422B -> 438B 0.58338
424B -> 438B -0.18819
425B -> 438B 0.11740

Excited State 66: 3.000-A 2.2177 eV 559.06 nm f=0.0000 <S**2>=2.000
435A -> 440A -0.18375
436A -> 440A 0.67574
435B -> 440B 0.18375
436B -> 440B -0.67574

Excited State 67: 1.000-A 2.2184 eV 558.88 nm f=0.0001 <S**2>=0.000
435A -> 440A -0.19318
436A -> 440A 0.67404
435B -> 440B -0.19318
436B -> 440B 0.67404

Excited State 68: 3.000-A 2.2337 eV 555.07 nm f=0.0000 <S**2>=2.000
397A -> 438A 0.11989
399A -> 438A 0.16957
409A -> 438A -0.12004
411A -> 438A -0.25300
417A -> 438A -0.10679
418A -> 438A 0.23230
419A -> 438A 0.17743
420A -> 438A 0.31835
421A -> 438A 0.11556
422A -> 438A 0.31126
397B -> 438B -0.11989
399B -> 438B -0.16957
409B -> 438B 0.12004
411B -> 438B 0.25300
417B -> 438B 0.10679
418B -> 438B -0.23230
419B -> 438B -0.17743
420B -> 438B -0.31835
421B -> 438B -0.11556

422B -> 438B -0.31126

Excited State 69: 1.000-A 2.2469 eV 551.81 nm f=0.0246 <S**2>=0.000
418A -> 437A 0.20335
419A -> 437A 0.15531
420A -> 437A -0.39822
421A -> 437A 0.47604
422A -> 437A 0.14931
418B -> 437B 0.20335
419B -> 437B 0.15531
420B -> 437B -0.39822
421B -> 437B 0.47604
422B -> 437B 0.14931

Excited State 70: 3.000-A 2.2522 eV 550.51 nm f=0.0000 <S**2>=2.000
410A -> 438A -0.11330
413A -> 438A 0.10964
415A -> 438A -0.16495
416A -> 438A 0.11661
418A -> 438A -0.14828
419A -> 438A -0.12586
420A -> 438A -0.12477
421A -> 438A 0.34378
422A -> 438A 0.36483
424A -> 438A -0.22124
425A -> 438A 0.19047
410B -> 438B 0.11330
413B -> 438B -0.10964
415B -> 438B 0.16495
416B -> 438B -0.11661
418B -> 438B 0.14828
419B -> 438B 0.12586
420B -> 438B 0.12477
421B -> 438B -0.34378
422B -> 438B -0.36483
424B -> 438B 0.22124

425B -> 438B -0.19047

Excited State 71: 1.000-A 2.2610 eV 548.37 nm f=0.0191 <S**2>=0.000
418A -> 438A 0.10122
419A -> 438A -0.29385
420A -> 438A 0.18674
421A -> 438A 0.50670
422A -> 438A 0.22671
424A -> 438A -0.13741
418B -> 438B 0.10122
419B -> 438B -0.29385
420B -> 438B 0.18674
421B -> 438B 0.50670
422B -> 438B 0.22671
424B -> 438B -0.13741

Excited State 72: 3.000-A 2.2648 eV 547.44 nm f=0.0000 <S**2>=2.000
434A -> 440A -0.17944
435A -> 440A -0.64785
436A -> 440A -0.17436
434B -> 440B 0.17944
435B -> 440B 0.64785
436B -> 440B 0.17436

Excited State 73: 3.000-A 2.2724 eV 545.60 nm f=0.0000 <S**2>=2.000
434A -> 439A 0.14074
435A -> 439A -0.68761
434B -> 439B -0.14074
435B -> 439B 0.68761

Excited State 74: 1.000-A 2.2736 eV 545.32 nm f=0.0003 <S**2>=0.000
434A -> 440A 0.16829
435A -> 440A 0.65233
436A -> 440A 0.18564
434B -> 440B 0.16829
435B -> 440B 0.65233

436B -> 440B 0.18564

Excited State 75: 1.000-A 2.2757 eV 544.81 nm f=0.0002 <S**2>=0.000
434A -> 439A -0.13748
435A -> 439A 0.68898
434B -> 439B -0.13748
435B -> 439B 0.68898

Excited State 76: 3.000-A 2.2851 eV 542.59 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.17004
403A -> 437A 0.35548
407A -> 437A 0.21395
409A -> 437A 0.10082
412A -> 437A 0.14069
416A -> 437A -0.12871
417A -> 437A -0.30723
418A -> 437A -0.29568
395B -> 437B -0.17004
403B -> 437B -0.35548
407B -> 437B -0.21395
409B -> 437B -0.10082
412B -> 437B -0.14069
416B -> 437B 0.12871
417B -> 437B 0.30723
418B -> 437B 0.29568

Excited State 77: 3.000-A 2.3165 eV 535.22 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.10356
401A -> 437A 0.14667
402A -> 437A 0.16004
403A -> 437A 0.16177
412A -> 437A 0.17663
413A -> 437A 0.14417
414A -> 437A -0.10668
415A -> 437A 0.20133
416A -> 437A -0.10145

417A -> 437A 0.33894
418A -> 437A 0.23094
420A -> 437A -0.23007
395B -> 437B 0.10356
401B -> 437B -0.14667
402B -> 437B -0.16004
403B -> 437B -0.16177
412B -> 437B -0.17663
413B -> 437B -0.14417
414B -> 437B 0.10668
415B -> 437B -0.20133
416B -> 437B 0.10145
417B -> 437B -0.33894
418B -> 437B -0.23094
420B -> 437B 0.23007

Excited State 78: 1.000-A 2.3258 eV 533.08 nm f=0.0057 <S**2>=0.000
412A -> 437A 0.10032
417A -> 437A 0.46305
418A -> 437A 0.44800
421A -> 437A -0.19844
412B -> 437B 0.10032
417B -> 437B 0.46305
418B -> 437B 0.44800
421B -> 437B -0.19844

Excited State 79: 1.000-A 2.3287 eV 532.42 nm f=0.0067 <S**2>=0.000
411A -> 438A -0.10949
418A -> 438A -0.10902
419A -> 438A 0.54410
420A -> 438A 0.22488
421A -> 438A 0.23420
422A -> 438A 0.13121
411B -> 438B -0.10949
418B -> 438B -0.10902
419B -> 438B 0.54410

420B -> 438B 0.22488
421B -> 438B 0.23420
422B -> 438B 0.13121

Excited State 80: 1.000-A 2.3499 eV 527.61 nm f=0.0001 <S**2>=0.000
423A -> 438A 0.70013
423B -> 438B 0.70013

Excited State 81: 3.000-A 2.3500 eV 527.60 nm f=0.0000 <S**2>=2.000
423A -> 438A -0.70308
423B -> 438B 0.70308

Excited State 82: 3.000-A 2.3564 eV 526.16 nm f=0.0000 <S**2>=2.000
397A -> 438A -0.17840
404A -> 438A 0.12069
405A -> 438A -0.10636
406A -> 438A 0.13646
408A -> 438A 0.10755
410A -> 438A 0.23834
413A -> 438A 0.11991
414A -> 438A -0.17088
415A -> 438A -0.15487
416A -> 438A 0.15073
418A -> 438A -0.15258
419A -> 438A 0.44968
397B -> 438B 0.17840
404B -> 438B -0.12069
405B -> 438B 0.10636
406B -> 438B -0.13646
408B -> 438B -0.10755
410B -> 438B -0.23834
413B -> 438B -0.11991
414B -> 438B 0.17088
415B -> 438B 0.15487
416B -> 438B -0.15073
418B -> 438B 0.15258

419B -> 438B -0.44968

Excited State 83: 3.000-A 2.3777 eV 521.44 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.13453
417A -> 437A -0.36378
418A -> 437A 0.40308
419A -> 437A 0.18012
420A -> 437A 0.24014
421A -> 437A -0.19699
395B -> 437B 0.13453
417B -> 437B 0.36378
418B -> 437B -0.40308
419B -> 437B -0.18012
420B -> 437B -0.24014
421B -> 437B 0.19699

Excited State 84: 1.000-A 2.3953 eV 517.61 nm f=0.0198 <S**2>=0.000
415A -> 438A 0.14291
417A -> 438A -0.12465
418A -> 438A 0.36090
420A -> 438A 0.48168
421A -> 438A -0.24308
415B -> 438B 0.14291
417B -> 438B -0.12465
418B -> 438B 0.36090
420B -> 438B 0.48168
421B -> 438B -0.24308

Excited State 85: 1.000-A 2.4038 eV 515.78 nm f=0.0117 <S**2>=0.000
417A -> 437A 0.43460
418A -> 437A -0.38620
419A -> 437A -0.19963
420A -> 437A -0.30275
417B -> 437B 0.43460
418B -> 437B -0.38620
419B -> 437B -0.19963

420B -> 437B -0.30275

Excited State 86: 3.000-A 2.4439 eV 507.32 nm f=0.0000 <S**2>=2.000
396A -> 438A -0.12830
397A -> 438A 0.44266
399A -> 438A 0.19994
402A -> 438A -0.13032
418A -> 438A -0.17463
419A -> 438A 0.15235
420A -> 438A -0.28362
396B -> 438B 0.12830
397B -> 438B -0.44266
399B -> 438B -0.19994
402B -> 438B 0.13032
418B -> 438B 0.17463
419B -> 438B -0.15235
420B -> 438B 0.28362

Excited State 87: 1.000-A 2.4457 eV 506.95 nm f=0.0149 <S**2>=0.000
415A -> 437A -0.20290
416A -> 437A 0.21001
417A -> 437A 0.23078
420A -> 437A 0.37042
421A -> 437A 0.40688
415B -> 437B -0.20290
416B -> 437B 0.21001
417B -> 437B 0.23078
420B -> 437B 0.37042
421B -> 437B 0.40688

Excited State 88: 3.000-A 2.4575 eV 504.51 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.45673
415A -> 437A 0.29328
416A -> 437A 0.21292
418A -> 437A 0.12972
420A -> 437A -0.12518

421A -> 437A -0.19680
395B -> 437B -0.45673
415B -> 437B -0.29328
416B -> 437B -0.21292
418B -> 437B -0.12972
420B -> 437B 0.12518
421B -> 437B 0.19680

Excited State 89: 3.000-A 2.4622 eV 503.55 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.12820
400A -> 437A 0.11607
412A -> 437A 0.10181
413A -> 437A 0.22284
416A -> 437A 0.12406
418A -> 437A 0.10738
420A -> 437A 0.40580
421A -> 437A 0.39629
422A -> 437A -0.12063
395B -> 437B -0.12820
400B -> 437B -0.11607
412B -> 437B -0.10181
413B -> 437B -0.22284
416B -> 437B -0.12406
418B -> 437B -0.10738
420B -> 437B -0.40580
421B -> 437B -0.39629
422B -> 437B 0.12063

Excited State 90: 1.000-A 2.4693 eV 502.10 nm f=0.0113 <S**2>=0.000
402A -> 438A -0.13792
404A -> 438A 0.13778
405A -> 438A -0.14385
406A -> 438A 0.15190
408A -> 438A 0.17025
409A -> 438A 0.15582
410A -> 438A 0.33183

411A -> 438A 0.19128
414A -> 438A -0.25509
417A -> 438A 0.10062
418A -> 438A -0.13739
419A -> 438A 0.24068
402B -> 438B -0.13792
404B -> 438B 0.13778
405B -> 438B -0.14385
406B -> 438B 0.15190
408B -> 438B 0.17025
409B -> 438B 0.15582
410B -> 438B 0.33183
411B -> 438B 0.19128
414B -> 438B -0.25509
417B -> 438B 0.10062
418B -> 438B -0.13739
419B -> 438B 0.24068

Excited State 91: 3.000-A 2.4833 eV 499.28 nm f=0.0000 <S**2>=2.000
410A -> 439A -0.14269
413A -> 439A -0.19670
414A -> 439A -0.61683
415A -> 439A -0.11773
416A -> 439A 0.12443
410B -> 439B 0.14269
413B -> 439B 0.19670
414B -> 439B 0.61683
415B -> 439B 0.11773
416B -> 439B -0.12443

Excited State 92: 3.000-A 2.4866 eV 498.61 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.12163
415A -> 440A 0.46447
416A -> 440A 0.44427
417A -> 440A -0.11013
418A -> 440A -0.13216

395B -> 437B 0.12163
415B -> 440B -0.46447
416B -> 440B -0.44427
417B -> 440B 0.11013
418B -> 440B 0.13216

Excited State 93: 1.000-A 2.5092 eV 494.12 nm f=0.0008 <S**2>=0.000
400A -> 437A 0.15422
402A -> 437A 0.21564
403A -> 437A -0.10010
404A -> 437A 0.16963
407A -> 437A -0.16748
412A -> 437A -0.15067
413A -> 437A 0.12149
415A -> 437A 0.37314
416A -> 437A 0.36426
400B -> 437B 0.15422
402B -> 437B 0.21564
403B -> 437B -0.10010
404B -> 437B 0.16963
407B -> 437B -0.16748
412B -> 437B -0.15067
413B -> 437B 0.12149
415B -> 437B 0.37314
416B -> 437B 0.36426

Excited State 94: 3.000-A 2.5296 eV 490.14 nm f=0.0000 <S**2>=2.000
397A -> 438A 0.30435
402A -> 438A -0.15046
405A -> 438A -0.10059
406A -> 438A 0.12136
409A -> 438A 0.12136
410A -> 438A -0.17929
411A -> 438A 0.15497
413A -> 438A 0.15257
420A -> 438A 0.35852

421A -> 438A -0.21252
397B -> 438B -0.30435
402B -> 438B 0.15046
405B -> 438B 0.10059
406B -> 438B -0.12136
409B -> 438B -0.12136
410B -> 438B 0.17929
411B -> 438B -0.15497
413B -> 438B -0.15257
420B -> 438B -0.35852
421B -> 438B 0.21252

Excited State 95: 1.000-A 2.5331 eV 489.45 nm f=0.0263 <S**2>=0.000
403A -> 437A 0.10535
412A -> 437A 0.14547
413A -> 437A 0.35779
414A -> 437A -0.22532
415A -> 437A 0.21691
416A -> 437A -0.33108
420A -> 437A 0.21063
421A -> 437A 0.19302
403B -> 437B 0.10535
412B -> 437B 0.14547
413B -> 437B 0.35779
414B -> 437B -0.22532
415B -> 437B 0.21691
416B -> 437B -0.33108
420B -> 437B 0.21063
421B -> 437B 0.19302

Excited State 96: 1.000-A 2.5513 eV 485.96 nm f=0.0147 <S**2>=0.000
410A -> 438A 0.18764
415A -> 438A -0.30144
416A -> 438A 0.33159
417A -> 438A -0.26127
418A -> 438A 0.30289

420A -> 438A -0.16960
410B -> 438B 0.18764
415B -> 438B -0.30144
416B -> 438B 0.33159
417B -> 438B -0.26127
418B -> 438B 0.30289
420B -> 438B -0.16960

Excited State 97: 3.000-A 2.5677 eV 482.86 nm f=0.0000 <S**2>=2.000
400A -> 438A 0.14108
411A -> 438A 0.30187
415A -> 438A -0.16592
416A -> 438A 0.19763
417A -> 438A -0.25980
418A -> 438A 0.38410
419A -> 438A 0.14336
420A -> 438A -0.11192
421A -> 438A 0.10454
400B -> 438B -0.14108
411B -> 438B -0.30187
415B -> 438B 0.16592
416B -> 438B -0.19763
417B -> 438B 0.25980
418B -> 438B -0.38410
419B -> 438B -0.14336
420B -> 438B 0.11192
421B -> 438B -0.10454

Excited State 98: 3.000-A 2.5769 eV 481.13 nm f=0.0000 <S**2>=2.000
411A -> 437A 0.28335
412A -> 437A -0.13938
413A -> 437A 0.33925
415A -> 437A -0.27933
416A -> 437A 0.18768
418A -> 437A 0.15242
419A -> 437A -0.28132

411B -> 437B -0.28335
412B -> 437B 0.13938
413B -> 437B -0.33925
415B -> 437B 0.27933
416B -> 437B -0.18768
418B -> 437B -0.15242
419B -> 437B 0.28132

Excited State 99: 1.000-A 2.5834 eV 479.93 nm f=0.0045 <S**2>=0.000
411A -> 437A -0.23192
412A -> 437A 0.24172
413A -> 437A -0.28074
415A -> 437A 0.37819
418A -> 437A -0.19786
419A -> 437A 0.24640
411B -> 437B -0.23192
412B -> 437B 0.24172
413B -> 437B -0.28074
415B -> 437B 0.37819
418B -> 437B -0.19786
419B -> 437B 0.24640

Excited State 100: 3.000-A 2.5853 eV 479.57 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.26357
412A -> 437A 0.15814
415A -> 437A 0.32382
416A -> 437A 0.43219
417A -> 437A -0.11007
419A -> 437A -0.12507
395B -> 437B 0.26357
412B -> 437B -0.15814
415B -> 437B -0.32382
416B -> 437B -0.43219
417B -> 437B 0.11007
419B -> 437B 0.12507

Excited State 101: 1.000-A 2.5917 eV 478.40 nm f=0.0035 <S**2>=0.000

| | |
|---|---|
| 400A -> 437A | 0.11711 |
| 402A -> 437A | 0.20589 |
| 404A -> 437A | 0.17823 |
| 407A -> 437A | -0.14682 |
| 412A -> 437A | -0.19178 |
| 413A -> 437A | -0.17680 |
| 415A -> 437A | -0.12344 |
| 416A -> 437A | -0.32596 |
| 417A -> 437A | 0.14145 |
| 419A -> 437A | 0.36225 |
| 400B -> 437B | 0.11711 |
| 402B -> 437B | 0.20589 |
| 404B -> 437B | 0.17823 |
| 407B -> 437B | -0.14682 |
| 412B -> 437B | -0.19178 |
| 413B -> 437B | -0.17680 |
| 415B -> 437B | -0.12344 |
| 416B -> 437B | -0.32596 |
| 417B -> 437B | 0.14145 |
| 419B -> 437B | 0.36225 |

Excited State 102: 1.000-A 2.5943 eV 477.90 nm f=0.0279 <S**2>=0.000

| | |
|---|---|
| 413A -> 438A | -0.21481 |
| 414A -> 438A | 0.18668 |
| 415A -> 438A | 0.25018 |
| 416A -> 438A | -0.22463 |
| 418A -> 438A | 0.33469 |
| 419A -> 438A | 0.18391 |
| 420A -> 438A | -0.30044 |
| 421A -> 438A | 0.15821 |
| 413B -> 438B | -0.21481 |
| 414B -> 438B | 0.18668 |
| 415B -> 438B | 0.25018 |
| 416B -> 438B | -0.22463 |
| 418B -> 438B | 0.33469 |

419B -> 438B 0.18391
420B -> 438B -0.30044
421B -> 438B 0.15821

Excited State 103: 3.000-A 2.6075 eV 475.49 nm f=0.0000 <S**2>=2.000
411A -> 437A 0.16765
413A -> 437A 0.15012
415A -> 437A -0.11085
416A -> 437A 0.18234
418A -> 437A -0.21991
419A -> 437A 0.56325
421A -> 437A -0.11979
411B -> 437B -0.16765
413B -> 437B -0.15012
415B -> 437B 0.11085
416B -> 437B -0.18234
418B -> 437B 0.21991
419B -> 437B -0.56325
421B -> 437B 0.11979

Excited State 104: 3.000-A 2.6103 eV 474.98 nm f=0.0000 <S**2>=2.000
431A -> 439A -0.21998
433A -> 439A 0.44589
434A -> 439A 0.45183
435A -> 439A 0.11782
436A -> 439A -0.13771
431B -> 439B 0.21998
433B -> 439B -0.44589
434B -> 439B -0.45183
435B -> 439B -0.11782
436B -> 439B 0.13771

Excited State 105: 1.000-A 2.6117 eV 474.73 nm f=0.0013 <S**2>=0.000
402A -> 437A -0.11104
404A -> 437A -0.10633
411A -> 437A 0.20016

413A -> 437A 0.26412
415A -> 437A -0.13989
416A -> 437A 0.20352
418A -> 437A -0.18852
419A -> 437A 0.46903
421A -> 437A -0.11876
402B -> 437B -0.11104
404B -> 437B -0.10633
411B -> 437B 0.20016
413B -> 437B 0.26412
415B -> 437B -0.13989
416B -> 437B 0.20352
418B -> 437B -0.18852
419B -> 437B 0.46903
421B -> 437B -0.11876

Excited State 106: 3.000-A 2.6142 eV 474.28 nm f=0.0000 <S**2>=2.000
430A -> 440A -0.20305
433A -> 440A -0.29281
434A -> 440A 0.55108
435A -> 440A -0.20772
430B -> 440B 0.20305
433B -> 440B 0.29281
434B -> 440B -0.55108
435B -> 440B 0.20772

Excited State 107: 3.000-A 2.6239 eV 472.51 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.10122
400A -> 437A 0.12569
409A -> 437A -0.22739
412A -> 437A 0.48879
413A -> 437A -0.14914
415A -> 437A -0.24457
416A -> 437A 0.12125
395B -> 437B -0.10122
400B -> 437B -0.12569

409B -> 437B 0.22739
412B -> 437B -0.48879
413B -> 437B 0.14914
415B -> 437B 0.24457
416B -> 437B -0.12125

Excited State 108: 1.000-A 2.6241 eV 472.48 nm f=0.0003 <S**2>=0.000
431A -> 439A -0.19884
433A -> 439A 0.44466
434A -> 439A 0.47966
435A -> 439A 0.11272
436A -> 439A -0.12437
431B -> 439B -0.19884
433B -> 439B 0.44466
434B -> 439B 0.47966
435B -> 439B 0.11272
436B -> 439B -0.12437

Excited State 109: 1.000-A 2.6300 eV 471.43 nm f=0.0002 <S**2>=0.000
430A -> 440A -0.17889
433A -> 440A -0.26127
434A -> 440A 0.59693
435A -> 440A -0.19034
430B -> 440B -0.17889
433B -> 440B -0.26127
434B -> 440B 0.59693
435B -> 440B -0.19034

Excited State 110: 1.000-A 2.6454 eV 468.67 nm f=0.0190 <S**2>=0.000
402A -> 437A 0.18097
403A -> 437A 0.15642
405A -> 437A -0.14366
411A -> 437A 0.22637
411A -> 438A 0.16158
412A -> 437A 0.43147
413A -> 438A -0.10462

414A -> 438A 0.10918
415A -> 437A -0.13446
402B -> 437B 0.18097
403B -> 437B 0.15642
405B -> 437B -0.14366
411B -> 437B 0.22637
411B -> 438B 0.16158
412B -> 437B 0.43147
413B -> 438B -0.10462
414B -> 438B 0.10918
415B -> 437B -0.13446

Excited State 111: 1.000-A 2.6470 eV 468.40 nm f=0.0020 <S**2>=0.000
410A -> 438A -0.13295
411A -> 438A 0.42550
412A -> 437A -0.17717
412A -> 438A 0.14032
413A -> 438A -0.21715
414A -> 438A 0.26101
415A -> 438A -0.12149
417A -> 438A -0.12433
410B -> 438B -0.13295
411B -> 438B 0.42550
412B -> 437B -0.17717
412B -> 438B 0.14032
413B -> 438B -0.21715
414B -> 438B 0.26101
415B -> 438B -0.12149
417B -> 438B -0.12433

Excited State 112: 3.000-A 2.6524 eV 467.43 nm f=0.0000 <S**2>=2.000
408A -> 438A -0.11172
410A -> 438A -0.14060
412A -> 438A -0.29394
413A -> 438A 0.37004
414A -> 438A -0.19794

415A -> 438A 0.18077
417A -> 438A 0.23386
418A -> 438A 0.25416
420A -> 438A -0.13645
408B -> 438B 0.11172
410B -> 438B 0.14060
412B -> 438B 0.29394
413B -> 438B -0.37004
414B -> 438B 0.19794
415B -> 438B -0.18077
417B -> 438B -0.23386
418B -> 438B -0.25416
420B -> 438B 0.13645

Excited State 113: 3.000-A 2.6586 eV 466.36 nm f=0.0000 <S**2>=2.000
404A -> 438A 0.11533
405A -> 438A -0.10714
406A -> 438A 0.11312
409A -> 438A 0.10877
413A -> 438A 0.14080
414A -> 438A 0.57726
415A -> 438A 0.14279
416A -> 438A -0.13775
404B -> 438B -0.11533
405B -> 438B 0.10714
406B -> 438B -0.11312
409B -> 438B -0.10877
413B -> 438B -0.14080
414B -> 438B -0.57726
415B -> 438B -0.14279
416B -> 438B 0.13775

Excited State 114: 1.000-A 2.6623 eV 465.71 nm f=0.0097 <S**2>=0.000
395A -> 437A -0.13103
403A -> 437A 0.25456
407A -> 437A 0.17335

408A -> 437A -0.11505
409A -> 437A 0.47278
410A -> 437A -0.13315
411A -> 437A -0.12378
412A -> 437A -0.19541
413A -> 437A 0.10153
436A -> 441A 0.11931
436A -> 443A 0.10553
395B -> 437B -0.13103
403B -> 437B 0.25456
407B -> 437B 0.17335
408B -> 437B -0.11505
409B -> 437B 0.47278
410B -> 437B -0.13315
411B -> 437B -0.12378
412B -> 437B -0.19541
413B -> 437B 0.10153
436B -> 441B 0.11931
436B -> 443B 0.10553

Excited State 115: 3.000-A 2.6671 eV 464.86 nm f=0.0000 <S**2>=2.000
409A -> 437A 0.12171
411A -> 437A -0.20226
413A -> 437A 0.13953
433A -> 443A 0.11608
435A -> 441A 0.22494
435A -> 443A 0.11402
436A -> 441A -0.36282
436A -> 442A -0.22544
436A -> 443A -0.18081
409B -> 437B -0.12171
411B -> 437B 0.20226
413B -> 437B -0.13953
433B -> 443B -0.11608
435B -> 441B -0.22494
435B -> 443B -0.11402

436B -> 441B 0.36282
436B -> 442B 0.22544
436B -> 443B 0.18081

Excited State 116: 1.000-A 2.6710 eV 464.18 nm f=0.0018 <S**2>=0.000
411A -> 438A 0.23672
412A -> 438A -0.29402
413A -> 438A 0.41403
414A -> 438A 0.16148
417A -> 438A 0.27964
418A -> 438A 0.15977
411B -> 438B 0.23672
412B -> 438B -0.29402
413B -> 438B 0.41403
414B -> 438B 0.16148
417B -> 438B 0.27964
418B -> 438B 0.15977

Excited State 117: 1.000-A 2.6732 eV 463.80 nm f=0.0051 <S**2>=0.000
408A -> 438A 0.15806
410A -> 438A 0.33758
411A -> 438A -0.14077
413A -> 438A 0.13531
414A -> 438A 0.50425
418A -> 438A -0.14932
408B -> 438B 0.15806
410B -> 438B 0.33758
411B -> 438B -0.14077
413B -> 438B 0.13531
414B -> 438B 0.50425
418B -> 438B -0.14932

Excited State 118: 3.000-A 2.6801 eV 462.61 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.13137
400A -> 437A -0.12064
409A -> 437A -0.25001

411A -> 437A 0.36131
413A -> 437A -0.19018
415A -> 437A 0.18850
433A -> 440A 0.12599
433A -> 442A -0.12552
435A -> 442A 0.11438
436A -> 441A -0.16676
436A -> 442A -0.14602
395B -> 437B 0.13137
400B -> 437B 0.12064
409B -> 437B 0.25001
411B -> 437B -0.36131
413B -> 437B 0.19018
415B -> 437B -0.18850
433B -> 440B -0.12599
433B -> 442B 0.12552
435B -> 442B -0.11438
436B -> 441B 0.16676
436B -> 442B 0.14602

Excited State 119: 3.000-A 2.6823 eV 462.23 nm f=0.0000 <S**2>=2.000
411A -> 437A 0.12342
433A -> 440A -0.51011
434A -> 440A -0.32909
435A -> 441A 0.11281
411B -> 437B -0.12342
433B -> 440B 0.51011
434B -> 440B 0.32909
435B -> 441B -0.11281

Excited State 120: 3.000-A 2.6844 eV 461.86 nm f=0.0000 <S**2>=2.000
400A -> 438A -0.11761
403A -> 438A -0.14956
404A -> 438A 0.14211
405A -> 438A -0.11961
407A -> 438A 0.11433

409A -> 438A 0.11758
410A -> 438A -0.24488
411A -> 438A -0.23658
412A -> 438A 0.26701
413A -> 438A -0.16331
414A -> 438A -0.20642
416A -> 438A -0.17903
417A -> 438A -0.14898
418A -> 438A 0.12766
420A -> 438A -0.12746
400B -> 438B 0.11761
403B -> 438B 0.14956
404B -> 438B -0.14211
405B -> 438B 0.11961
407B -> 438B -0.11433
409B -> 438B -0.11758
410B -> 438B 0.24488
411B -> 438B 0.23658
412B -> 438B -0.26701
413B -> 438B 0.16331
414B -> 438B 0.20642
416B -> 438B 0.17903
417B -> 438B 0.14898
418B -> 438B -0.12766
420B -> 438B 0.12746

Excited State 121: 1.000-A 2.6853 eV 461.72 nm f=0.0000 <S**2>=0.000
433A -> 440A 0.62509
434A -> 440A 0.29730
433B -> 440B 0.62509
434B -> 440B 0.29730

Excited State 122: 1.000-A 2.6876 eV 461.32 nm f=0.0021 <S**2>=0.000
400A -> 437A -0.18773
403A -> 437A 0.14356
407A -> 437A 0.19160

408A -> 437A -0.10462
409A -> 437A -0.16622
411A -> 437A 0.40774
412A -> 437A -0.24041
413A -> 437A -0.21070
415A -> 437A 0.19603
400B -> 437B -0.18773
403B -> 437B 0.14356
407B -> 437B 0.19160
408B -> 437B -0.10462
409B -> 437B -0.16622
411B -> 437B 0.40774
412B -> 437B -0.24041
413B -> 437B -0.21070
415B -> 437B 0.19603

Excited State 123: 3.000-A 2.6910 eV 460.74 nm f=0.0000 <S**2>=2.000
430A -> 441A 0.16409
430A -> 442A -0.14225
433A -> 440A -0.28494
433A -> 441A 0.16701
433A -> 442A -0.10448
434A -> 441A -0.16939
434A -> 442A 0.17846
435A -> 441A -0.22965
435A -> 442A 0.20806
435A -> 443A 0.14902
436A -> 441A -0.13671
436A -> 442A 0.13161
430B -> 441B -0.16409
430B -> 442B 0.14225
433B -> 440B 0.28494
433B -> 441B -0.16701
433B -> 442B 0.10448
434B -> 441B 0.16939
434B -> 442B -0.17846

435B -> 441B 0.22965
435B -> 442B -0.20806
435B -> 443B -0.14902
436B -> 441B 0.13671
436B -> 442B -0.13161

Excited State 124: 3.000-A 2.6929 eV 460.41 nm f=0.0000 <S**2>=2.000
411A -> 437A 0.12393
415A -> 437A 0.10522
431A -> 442A -0.12972
433A -> 441A 0.11009
433A -> 442A 0.19534
434A -> 441A 0.13677
434A -> 442A 0.12563
435A -> 441A 0.12562
435A -> 442A -0.11332
435A -> 443A 0.17193
436A -> 442A 0.20387
436A -> 443A -0.37658
411B -> 437B -0.12393
415B -> 437B -0.10522
431B -> 442B 0.12972
433B -> 441B -0.11009
433B -> 442B -0.19534
434B -> 441B -0.13677
434B -> 442B -0.12563
435B -> 441B -0.12562
435B -> 442B 0.11332
435B -> 443B -0.17193
436B -> 442B -0.20387
436B -> 443B 0.37658

Excited State 125: 3.000-A 2.7056 eV 458.25 nm f=0.0000 <S**2>=2.000
433A -> 439A -0.48013
434A -> 439A 0.48950
433B -> 439B 0.48013

434B -> 439B -0.48950

Excited State 126: 1.000-A 2.7068 eV 458.04 nm f=0.0001 <S**2>=0.000
433A -> 439A 0.49640
434A -> 439A -0.47935
433B -> 439B 0.49640
434B -> 439B -0.47935

Excited State 127: 3.000-A 2.7079 eV 457.85 nm f=0.0000 <S**2>=2.000
413A -> 438A -0.29909
415A -> 438A -0.18187
416A -> 438A 0.14193
417A -> 438A 0.51960
418A -> 438A 0.21849
413B -> 438B 0.29909
415B -> 438B 0.18187
416B -> 438B -0.14193
417B -> 438B -0.51960
418B -> 438B -0.21849

Excited State 128: 1.000-A 2.7095 eV 457.58 nm f=0.0011 <S**2>=0.000
411A -> 438A -0.11733
413A -> 438A -0.30910
414A -> 438A 0.10714
415A -> 438A -0.20054
416A -> 438A 0.16038
417A -> 438A 0.49873
418A -> 438A 0.16689
411B -> 438B -0.11733
413B -> 438B -0.30910
414B -> 438B 0.10714
415B -> 438B -0.20054
416B -> 438B 0.16038
417B -> 438B 0.49873
418B -> 438B 0.16689

Excited State 129: 3.000-A 2.7157 eV 456.55 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 398A -> 437A | -0.11375 |
| 401A -> 437A | -0.15540 |
| 403A -> 437A | -0.23212 |
| 408A -> 437A | -0.12828 |
| 409A -> 437A | 0.39804 |
| 410A -> 437A | -0.27725 |
| 411A -> 437A | 0.15379 |
| 412A -> 437A | 0.23384 |
| 414A -> 437A | 0.19507 |
| 398B -> 437B | 0.11375 |
| 401B -> 437B | 0.15540 |
| 403B -> 437B | 0.23212 |
| 408B -> 437B | 0.12828 |
| 409B -> 437B | -0.39804 |
| 410B -> 437B | 0.27725 |
| 411B -> 437B | -0.15379 |
| 412B -> 437B | -0.23384 |
| 414B -> 437B | -0.19507 |

Excited State 130: 1.000-A 2.7281 eV 454.47 nm f=0.0017 <S**2>=0.000

| | |
|---|---|
| 403A -> 437A | -0.23238 |
| 409A -> 437A | 0.19534 |
| 410A -> 437A | -0.21580 |
| 411A -> 437A | 0.16646 |
| 412A -> 437A | 0.10791 |
| 414A -> 437A | 0.50748 |
| 416A -> 437A | -0.12410 |
| 403B -> 437B | -0.23238 |
| 409B -> 437B | 0.19534 |
| 410B -> 437B | -0.21580 |
| 411B -> 437B | 0.16646 |
| 412B -> 437B | 0.10791 |
| 414B -> 437B | 0.50748 |
| 416B -> 437B | -0.12410 |

Excited State 131: 3.000-A 2.7337 eV 453.53 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 401A -> 437A | 0.10514 |
| 409A -> 437A | -0.16233 |
| 413A -> 437A | 0.22580 |
| 414A -> 437A | 0.60554 |
| 401B -> 437B | -0.10514 |
| 409B -> 437B | 0.16233 |
| 413B -> 437B | -0.22580 |
| 414B -> 437B | -0.60554 |

Excited State 132: 1.000-A 2.7371 eV 452.98 nm f=0.0155 <S**2>=0.000

| | |
|---|---|
| 402A -> 438A | 0.11557 |
| 407A -> 438A | 0.12297 |
| 408A -> 438A | -0.10744 |
| 412A -> 438A | 0.48464 |
| 413A -> 438A | 0.19839 |
| 416A -> 438A | -0.24888 |
| 417A -> 438A | 0.17000 |
| 418A -> 438A | 0.17356 |
| 402B -> 438B | 0.11557 |
| 407B -> 438B | 0.12297 |
| 408B -> 438B | -0.10744 |
| 412B -> 438B | 0.48464 |
| 413B -> 438B | 0.19839 |
| 416B -> 438B | -0.24888 |
| 417B -> 438B | 0.17000 |
| 418B -> 438B | 0.17356 |

Excited State 133: 3.000-A 2.7377 eV 452.88 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 402A -> 438A | 0.16042 |
| 408A -> 438A | -0.11875 |
| 410A -> 438A | 0.22517 |
| 411A -> 438A | 0.17986 |
| 412A -> 438A | 0.40734 |
| 413A -> 438A | 0.21036 |
| 416A -> 438A | -0.22594 |

417A -> 438A 0.17101
418A -> 438A 0.13505
402B -> 438B -0.16042
408B -> 438B 0.11875
410B -> 438B -0.22517
411B -> 438B -0.17986
412B -> 438B -0.40734
413B -> 438B -0.21036
416B -> 438B 0.22594
417B -> 438B -0.17101
418B -> 438B -0.13505

Excited State 134: 1.000-A 2.7403 eV 452.45 nm f=0.0015 <S**2>=0.000
403A -> 437A 0.25187
405A -> 437A -0.10460
407A -> 437A 0.12033
409A -> 437A -0.33850
411A -> 437A -0.18853
413A -> 437A 0.24577
414A -> 437A 0.37908
403B -> 437B 0.25187
405B -> 437B -0.10460
407B -> 437B 0.12033
409B -> 437B -0.33850
411B -> 437B -0.18853
413B -> 437B 0.24577
414B -> 437B 0.37908

Excited State 135: 3.000-A 2.7469 eV 451.36 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.12821
399A -> 437A 0.13857
401A -> 437A 0.24967
404A -> 437A -0.11257
405A -> 437A 0.23849
406A -> 437A -0.14600
407A -> 437A -0.14068

408A -> 437A 0.31257
409A -> 437A 0.16280
411A -> 437A 0.28099
416A -> 437A -0.11695
398B -> 437B -0.12821
399B -> 437B -0.13857
401B -> 437B -0.24967
404B -> 437B 0.11257
405B -> 437B -0.23849
406B -> 437B 0.14600
407B -> 437B 0.14068
408B -> 437B -0.31257
409B -> 437B -0.16280
411B -> 437B -0.28099
416B -> 437B 0.11695

Excited State 136: 1.000-A 2.7551 eV 450.01 nm f=0.0127 <S**2>=0.000
402A -> 438A 0.15838
403A -> 438A 0.16697
404A -> 438A -0.25610
405A -> 438A 0.22707
406A -> 438A -0.21988
409A -> 438A -0.20097
410A -> 438A 0.33939
411A -> 438A 0.23873
402B -> 438B 0.15838
403B -> 438B 0.16697
404B -> 438B -0.25610
405B -> 438B 0.22707
406B -> 438B -0.21988
409B -> 438B -0.20097
410B -> 438B 0.33939
411B -> 438B 0.23873

Excited State 137: 3.000-A 2.7686 eV 447.81 nm f=0.0000 <S**2>=2.000
397A -> 438A -0.11366

410A -> 438A -0.11910
411A -> 438A 0.10677
415A -> 438A 0.12153
434A -> 444A 0.11491
435A -> 443A -0.19439
435A -> 444A -0.41384
436A -> 443A -0.12399
436A -> 444A -0.32212
397B -> 438B 0.11366
410B -> 438B 0.11910
411B -> 438B -0.10677
415B -> 438B -0.12153
434B -> 444B -0.11491
435B -> 443B 0.19439
435B -> 444B 0.41384
436B -> 443B 0.12399
436B -> 444B 0.32212

Excited State 138: 1.000-A 2.7699 eV 447.61 nm f=0.0006 <S**2>=0.000
401A -> 437A 0.29174
403A -> 437A 0.23491
405A -> 437A 0.14987
406A -> 437A -0.14639
407A -> 437A -0.23361
408A -> 437A 0.34702
410A -> 437A 0.17803
411A -> 437A 0.23760
401B -> 437B 0.29174
403B -> 437B 0.23491
405B -> 437B 0.14987
406B -> 437B -0.14639
407B -> 437B -0.23361
408B -> 437B 0.34702
410B -> 437B 0.17803
411B -> 437B 0.23760

Excited State 139: 3.000-A 2.7744 eV 446.88 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 399A -> 438A | 0.16065 |
| 400A -> 438A | -0.20343 |
| 401A -> 438A | -0.15281 |
| 402A -> 438A | 0.21866 |
| 403A -> 438A | -0.12974 |
| 407A -> 438A | 0.11741 |
| 408A -> 438A | -0.17661 |
| 409A -> 438A | 0.19319 |
| 415A -> 438A | 0.23898 |
| 416A -> 438A | 0.35261 |
| 435A -> 444A | 0.13951 |
| 436A -> 444A | 0.10338 |
| 399B -> 438B | -0.16065 |
| 400B -> 438B | 0.20343 |
| 401B -> 438B | 0.15281 |
| 402B -> 438B | -0.21866 |
| 403B -> 438B | 0.12974 |
| 407B -> 438B | -0.11741 |
| 408B -> 438B | 0.17661 |
| 409B -> 438B | -0.19319 |
| 415B -> 438B | -0.23898 |
| 416B -> 438B | -0.35261 |
| 435B -> 444B | -0.13951 |
| 436B -> 444B | -0.10338 |

Excited State 140: 1.000-A 2.7814 eV 445.77 nm f=0.0014 <S**2>=0.000

| | |
|---|---|
| 402A -> 438A | 0.14657 |
| 408A -> 438A | -0.15282 |
| 409A -> 438A | 0.12544 |
| 410A -> 438A | 0.12193 |
| 412A -> 438A | 0.15002 |
| 415A -> 438A | 0.42334 |
| 416A -> 438A | 0.42468 |
| 402B -> 438B | 0.14657 |
| 408B -> 438B | -0.15282 |

409B -> 438B 0.12544
410B -> 438B 0.12193
412B -> 438B 0.15002
415B -> 438B 0.42334
416B -> 438B 0.42468

Excited State 141: 3.000-A 2.7913 eV 444.18 nm f=0.0000 <S**2>=2.000
399A -> 438A -0.14968
400A -> 438A 0.22518
401A -> 438A 0.11404
402A -> 438A -0.14816
403A -> 438A 0.13268
409A -> 438A -0.13178
412A -> 438A 0.29591
415A -> 438A 0.38863
416A -> 438A 0.28296
399B -> 438B 0.14968
400B -> 438B -0.22518
401B -> 438B -0.11404
402B -> 438B 0.14816
403B -> 438B -0.13268
409B -> 438B 0.13178
412B -> 438B -0.29591
415B -> 438B -0.38863
416B -> 438B -0.28296

Excited State 142: 3.000-A 2.7944 eV 443.70 nm f=0.0000 <S**2>=2.000
394A -> 437A 0.10970
398A -> 437A 0.15177
399A -> 437A 0.15864
402A -> 437A 0.19463
403A -> 437A -0.29757
404A -> 437A -0.16691
405A -> 437A 0.10550
407A -> 437A 0.45796
408A -> 437A -0.10877

394B -> 437B -0.10970
398B -> 437B -0.15177
399B -> 437B -0.15864
402B -> 437B -0.19463
403B -> 437B 0.29757
404B -> 437B 0.16691
405B -> 437B -0.10550
407B -> 437B -0.45796
408B -> 437B 0.10877

Excited State 143: 1.000-A 2.8111 eV 441.05 nm f=0.0038 <S**2>=0.000
400A -> 438A 0.23494
401A -> 438A 0.15061
402A -> 438A -0.20714
403A -> 438A 0.15806
407A -> 438A -0.12266
408A -> 438A 0.26407
409A -> 438A -0.25223
412A -> 438A 0.28614
413A -> 438A 0.11485
415A -> 438A 0.21510
416A -> 438A 0.11583
400B -> 438B 0.23494
401B -> 438B 0.15061
402B -> 438B -0.20714
403B -> 438B 0.15806
407B -> 438B -0.12266
408B -> 438B 0.26407
409B -> 438B -0.25223
412B -> 438B 0.28614
413B -> 438B 0.11485
415B -> 438B 0.21510
416B -> 438B 0.11583

Excited State 144: 3.000-A 2.8154 eV 440.38 nm f=0.0000 <S**2>=2.000
398A -> 438A 0.11753

399A -> 438A -0.15461
401A -> 437A -0.27446
401A -> 438A 0.12342
404A -> 437A 0.13729
405A -> 437A 0.24580
408A -> 437A -0.15642
410A -> 437A 0.34003
410A -> 438A 0.14688
411A -> 438A -0.10925
398B -> 438B -0.11753
399B -> 438B 0.15461
401B -> 437B 0.27446
401B -> 438B -0.12342
404B -> 437B -0.13729
405B -> 437B -0.24580
408B -> 437B 0.15642
410B -> 437B -0.34003
410B -> 438B -0.14688
411B -> 438B 0.10925

Excited State 145: 3.000-A 2.8177 eV 440.02 nm f=0.0000 <S**2>=2.000
397A -> 438A 0.13248
398A -> 438A 0.18480
399A -> 438A -0.23093
401A -> 437A 0.21603
401A -> 438A 0.14315
404A -> 437A -0.11775
404A -> 438A -0.10641
405A -> 437A -0.15563
405A -> 438A 0.14065
408A -> 438A -0.14048
409A -> 438A 0.13396
410A -> 437A -0.18297
410A -> 438A 0.27178
411A -> 438A -0.15201
397B -> 438B -0.13248

398B -> 438B -0.18480
399B -> 438B 0.23093
401B -> 437B -0.21603
401B -> 438B -0.14315
404B -> 437B 0.11775
404B -> 438B 0.10641
405B -> 437B 0.15563
405B -> 438B -0.14065
408B -> 438B 0.14048
409B -> 438B -0.13396
410B -> 437B 0.18297
410B -> 438B -0.27178
411B -> 438B 0.15201

Excited State 146: 1.000-A 2.8198 eV 439.69 nm f=0.0029 <S**2>=0.000
401A -> 437A 0.41572
403A -> 437A -0.24098
404A -> 437A -0.27060
405A -> 437A -0.18280
407A -> 437A 0.21005
408A -> 437A 0.17195
410A -> 437A -0.19818
401B -> 437B 0.41572
403B -> 437B -0.24098
404B -> 437B -0.27060
405B -> 437B -0.18280
407B -> 437B 0.21005
408B -> 437B 0.17195
410B -> 437B -0.19818

Excited State 147: 1.000-A 2.8273 eV 438.52 nm f=0.0005 <S**2>=0.000
400A -> 437A 0.12310
402A -> 437A 0.16534
403A -> 437A -0.16688
405A -> 437A 0.16955
407A -> 437A 0.33358

408A -> 437A -0.14135
410A -> 437A 0.46290
411A -> 437A 0.11044
400B -> 437B 0.12310
402B -> 437B 0.16534
403B -> 437B -0.16688
405B -> 437B 0.16955
407B -> 437B 0.33358
408B -> 437B -0.14135
410B -> 437B 0.46290
411B -> 437B 0.11044

Excited State 148: 3.000-A 2.8390 eV 436.72 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.11062
403A -> 437A -0.11445
404A -> 437A -0.25300
405A -> 437A -0.36187
408A -> 437A -0.11038
408A -> 438A -0.10128
409A -> 437A 0.14588
410A -> 437A 0.42285
398B -> 437B 0.11062
403B -> 437B 0.11445
404B -> 437B 0.25300
405B -> 437B 0.36187
408B -> 437B 0.11038
408B -> 438B 0.10128
409B -> 437B -0.14588
410B -> 437B -0.42285

Excited State 149: 3.000-A 2.8416 eV 436.32 nm f=0.0000 <S**2>=2.000
400A -> 438A -0.14375
401A -> 438A 0.24503
403A -> 438A -0.12139
405A -> 438A 0.17538
406A -> 438A -0.13111

408A -> 438A 0.46173
410A -> 438A -0.12970
411A -> 438A 0.11812
413A -> 438A 0.13203
400B -> 438B 0.14375
401B -> 438B -0.24503
403B -> 438B 0.12139
405B -> 438B -0.17538
406B -> 438B 0.13111
408B -> 438B -0.46173
410B -> 438B 0.12970
411B -> 438B -0.11812
413B -> 438B -0.13203

Excited State 150: 1.000-A 2.8459 eV 435.66 nm f=0.0008 <S**2>=0.000
404A -> 437A 0.28752
405A -> 437A 0.47797
407A -> 437A 0.24533
408A -> 437A 0.11006
409A -> 437A -0.11350
410A -> 437A -0.28325
404B -> 437B 0.28752
405B -> 437B 0.47797
407B -> 437B 0.24533
408B -> 437B 0.11006
409B -> 437B -0.11350
410B -> 437B -0.28325

Excited State 151: 1.000-A 2.8592 eV 433.64 nm f=0.0037 <S**2>=0.000
397A -> 438A -0.15610
400A -> 438A -0.16796
402A -> 438A 0.22666
403A -> 438A -0.10700
406A -> 438A -0.15471
407A -> 438A 0.16305
408A -> 438A 0.50021

410A -> 438A -0.12717
411A -> 438A 0.11922
397B -> 438B -0.15610
400B -> 438B -0.16796
402B -> 438B 0.22666
403B -> 438B -0.10700
406B -> 438B -0.15471
407B -> 438B 0.16305
408B -> 438B 0.50021
410B -> 438B -0.12717
411B -> 438B 0.11922

Excited State 152: 3.000-A 2.8707 eV 431.89 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.21867
399A -> 437A -0.12507
400A -> 437A 0.13689
401A -> 437A 0.31807
402A -> 437A -0.16697
403A -> 437A -0.10162
404A -> 437A 0.30165
405A -> 437A 0.14568
407A -> 437A 0.21121
435A -> 445A 0.10095
398B -> 437B 0.21867
399B -> 437B 0.12507
400B -> 437B -0.13689
401B -> 437B -0.31807
402B -> 437B 0.16697
403B -> 437B 0.10162
404B -> 437B -0.30165
405B -> 437B -0.14568
407B -> 437B -0.21121
435B -> 445B -0.10095

Excited State 153: 1.000-A 2.8763 eV 431.05 nm f=0.0074 <S**2>=0.000
399A -> 438A -0.20504

401A -> 438A 0.45106
402A -> 438A -0.10931
404A -> 438A -0.14161
405A -> 438A 0.17113
406A -> 438A 0.13987
407A -> 438A -0.24819
409A -> 438A 0.25703
399B -> 438B -0.20504
401B -> 438B 0.45106
402B -> 438B -0.10931
404B -> 438B -0.14161
405B -> 438B 0.17113
406B -> 438B 0.13987
407B -> 438B -0.24819
409B -> 438B 0.25703

Excited State 154: 3.000-A 2.8767 eV 430.99 nm f=0.0000 <S**2>=2.000
393A -> 440A -0.12820
401A -> 437A 0.15360
401A -> 438A 0.12246
404A -> 437A 0.15267
406A -> 438A 0.12660
407A -> 438A -0.14320
408A -> 438A -0.11547
432A -> 440A 0.25777
433A -> 445A 0.11014
434A -> 445A -0.13353
435A -> 445A -0.19694
436A -> 442A -0.10391
436A -> 445A -0.13207
393B -> 440B 0.12820
401B -> 437B -0.15360
401B -> 438B -0.12246
404B -> 437B -0.15267
406B -> 438B -0.12660
407B -> 438B 0.14320

408B -> 438B 0.11547
432B -> 440B -0.25777
433B -> 445B -0.11014
434B -> 445B 0.13353
435B -> 445B 0.19694
436B -> 442B 0.10391
436B -> 445B 0.13207

Excited State 155: 3.000-A 2.8830 eV 430.05 nm f=0.0000 <S**2>=2.000
393A -> 440A -0.21378
398A -> 438A 0.15434
400A -> 438A 0.13065
401A -> 438A -0.24920
406A -> 438A -0.24763
407A -> 438A 0.26500
408A -> 438A 0.10972
432A -> 440A 0.32682
393B -> 440B 0.21378
398B -> 438B -0.15434
400B -> 438B -0.13065
401B -> 438B 0.24920
406B -> 438B 0.24763
407B -> 438B -0.26500
408B -> 438B -0.10972
432B -> 440B -0.32682

Excited State 156: 3.000-A 2.8840 eV 429.90 nm f=0.0000 <S**2>=2.000
392A -> 439A 0.21967
393A -> 440A -0.17700
401A -> 438A 0.15472
406A -> 438A 0.14351
407A -> 438A -0.15807
431A -> 439A 0.13144
432A -> 439A 0.25878
432A -> 440A 0.22601
435A -> 445A 0.10938

392B -> 439B -0.21967
393B -> 440B 0.17700
401B -> 438B -0.15472
406B -> 438B -0.14351
407B -> 438B 0.15807
431B -> 439B -0.13144
432B -> 439B -0.25878
432B -> 440B -0.22601
435B -> 445B -0.10938

Excited State 157: 3.000-A 2.8854 eV 429.70 nm f=0.0000 <S**2>=2.000
392A -> 439A 0.31775
393A -> 440A 0.14412
431A -> 439A 0.18990
432A -> 439A 0.35571
432A -> 440A -0.17320
435A -> 445A -0.11527
392B -> 439B -0.31775
393B -> 440B -0.14412
431B -> 439B -0.18990
432B -> 439B -0.35571
432B -> 440B 0.17320
435B -> 445B 0.11527

Excited State 158: 3.000-A 2.8912 eV 428.83 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.54982
402A -> 437A -0.14448
404A -> 437A -0.16784
408A -> 437A 0.14219
410A -> 437A -0.13184
412A -> 437A -0.11076
400B -> 437B -0.54982
402B -> 437B 0.14448
404B -> 437B 0.16784
408B -> 437B -0.14219
410B -> 437B 0.13184

412B -> 437B 0.11076

Excited State 159: 1.000-A 2.8946 eV 428.34 nm f=0.0121 <S**2>=0.000
395A -> 437A -0.23218
398A -> 437A -0.12385
399A -> 437A -0.16874
400A -> 437A -0.32545
401A -> 437A 0.21759
404A -> 437A 0.34181
408A -> 437A -0.12871
410A -> 437A 0.14057
436A -> 441A -0.17435
436A -> 443A -0.10804
395B -> 437B -0.23218
398B -> 437B -0.12385
399B -> 437B -0.16874
400B -> 437B -0.32545
401B -> 437B 0.21759
404B -> 437B 0.34181
408B -> 437B -0.12871
410B -> 437B 0.14057
436B -> 441B -0.17435
436B -> 443B -0.10804

Excited State 160: 1.000-A 2.9058 eV 426.68 nm f=0.0007 <S**2>=0.000
432A -> 440A 0.69156
432B -> 440B 0.69156

Excited State 161: 1.000-A 2.9073 eV 426.45 nm f=0.0005 <S**2>=0.000
397A -> 438A -0.14547
399A -> 438A 0.14621
400A -> 438A -0.14887
402A -> 438A 0.12841
406A -> 437A 0.24576
406A -> 438A 0.46076
407A -> 438A -0.11380

409A -> 438A -0.27852
397B -> 438B -0.14547
399B -> 438B 0.14621
400B -> 438B -0.14887
402B -> 438B 0.12841
406B -> 437B 0.24576
406B -> 438B 0.46076
407B -> 438B -0.11380
409B -> 438B -0.27852

Excited State 162: 3.000-A 2.9100 eV 426.06 nm f=0.0000 <S**2>=2.000
401A -> 437A 0.10103
404A -> 437A -0.19991
405A -> 437A 0.22438
406A -> 437A 0.49988
407A -> 437A -0.20588
408A -> 437A -0.17762
432A -> 439A -0.10661
401B -> 437B -0.10103
404B -> 437B 0.19991
405B -> 437B -0.22438
406B -> 437B -0.49988
407B -> 437B 0.20588
408B -> 437B 0.17762
432B -> 439B 0.10661

Excited State 163: 3.000-A 2.9108 eV 425.94 nm f=0.0000 <S**2>=2.000
393A -> 440A 0.43266
407A -> 440A -0.10051
432A -> 440A 0.43357
393B -> 440B -0.43266
407B -> 440B 0.10051
432B -> 440B -0.43357

Excited State 164: 1.000-A 2.9116 eV 425.83 nm f=0.0004 <S**2>=0.000
395A -> 437A 0.10126

401A -> 437A 0.17422
402A -> 437A -0.15515
405A -> 437A 0.15779
406A -> 437A 0.51647
406A -> 438A -0.20874
407A -> 437A -0.13922
409A -> 438A 0.12066
395B -> 437B 0.10126
401B -> 437B 0.17422
402B -> 437B -0.15515
405B -> 437B 0.15779
406B -> 437B 0.51647
406B -> 438B -0.20874
407B -> 437B -0.13922
409B -> 438B 0.12066

Excited State 165: 1.000-A 2.9120 eV 425.76 nm f=0.0006 <S**2>=0.000
429A -> 439A 0.11779
431A -> 439A 0.10218
432A -> 439A 0.68090
429B -> 439B 0.11779
431B -> 439B 0.10218
432B -> 439B 0.68090

Excited State 166: 3.000-A 2.9124 eV 425.72 nm f=0.0000 <S**2>=2.000
392A -> 439A -0.37499
406A -> 437A 0.13258
408A -> 439A 0.11160
432A -> 439A 0.47485
392B -> 439B 0.37499
406B -> 437B -0.13258
408B -> 439B -0.11160
432B -> 439B -0.47485

Excited State 167: 3.000-A 2.9171 eV 425.03 nm f=0.0000 <S**2>=2.000
400A -> 438A 0.20781

401A -> 438A -0.19596
403A -> 438A 0.14103
404A -> 438A -0.22100
405A -> 438A 0.23745
406A -> 438A 0.27520
408A -> 437A 0.15217
408A -> 438A 0.10056
409A -> 438A 0.29755
411A -> 438A -0.14329
400B -> 438B -0.20781
401B -> 438B 0.19596
403B -> 438B -0.14103
404B -> 438B 0.22100
405B -> 438B -0.23745
406B -> 438B -0.27520
408B -> 437B -0.15217
408B -> 438B -0.10056
409B -> 438B -0.29755
411B -> 438B 0.14329

Excited State 168: 1.000-A 2.9172 eV 425.01 nm f=0.0020 <S**2>=0.000
398A -> 437A -0.18689
399A -> 437A -0.13644
400A -> 437A 0.31570
402A -> 437A -0.23636
404A -> 437A 0.26637
405A -> 437A -0.21951
407A -> 437A 0.18145
408A -> 437A 0.28234
409A -> 437A 0.10234
398B -> 437B -0.18689
399B -> 437B -0.13644
400B -> 437B 0.31570
402B -> 437B -0.23636
404B -> 437B 0.26637
405B -> 437B -0.21951

407B -> 437B 0.18145
408B -> 437B 0.28234
409B -> 437B 0.10234

Excited State 169: 3.000-A 2.9192 eV 424.72 nm f=0.0000 <S**2>=2.000
401A -> 437A -0.15354
404A -> 437A 0.13737
405A -> 437A -0.11337
406A -> 437A 0.38149
408A -> 437A 0.38859
409A -> 437A 0.10732
409A -> 438A -0.13876
401B -> 437B 0.15354
404B -> 437B -0.13737
405B -> 437B 0.11337
406B -> 437B -0.38149
408B -> 437B -0.38859
409B -> 437B -0.10732
409B -> 438B 0.13876

Excited State 170: 1.000-A 2.9214 eV 424.40 nm f=0.0127 <S**2>=0.000
395A -> 437A 0.20975
397A -> 438A 0.15878
399A -> 438A 0.17913
400A -> 437A -0.21895
401A -> 438A -0.12133
404A -> 438A -0.14538
405A -> 438A 0.20058
406A -> 437A -0.13210
409A -> 438A 0.17535
435A -> 444A 0.10075
436A -> 441A 0.27253
436A -> 443A 0.18482
395B -> 437B 0.20975
397B -> 438B 0.15878
399B -> 438B 0.17913

400B -> 437B -0.21895
401B -> 438B -0.12133
404B -> 438B -0.14538
405B -> 438B 0.20058
406B -> 437B -0.13210
409B -> 438B 0.17535
435B -> 444B 0.10075
436B -> 441B 0.27253
436B -> 443B 0.18482

Excited State 171: 1.000-A 2.9234 eV 424.11 nm f=0.0217 <S**2>=0.000
395A -> 437A 0.20866
397A -> 438A -0.13098
399A -> 438A -0.15137
400A -> 437A -0.23174
400A -> 438A -0.10860
401A -> 438A 0.16866
403A -> 438A -0.11287
404A -> 438A 0.15796
405A -> 438A -0.20757
406A -> 438A -0.12201
408A -> 438A -0.10622
409A -> 438A -0.19743
436A -> 441A 0.26833
395B -> 437B 0.20866
397B -> 438B -0.13098
399B -> 438B -0.15137
400B -> 437B -0.23174
400B -> 438B -0.10860
401B -> 438B 0.16866
403B -> 438B -0.11287
404B -> 438B 0.15796
405B -> 438B -0.20757
406B -> 438B -0.12201
408B -> 438B -0.10622
409B -> 438B -0.19743

436B -> 441B 0.26833

Excited State 172: 3.000-A 2.9235 eV 424.09 nm f=0.0000 <S**2>=2.000
406A -> 437A -0.10701
408A -> 437A -0.17888
431A -> 442A 0.10516
432A -> 439A -0.10086
433A -> 448A 0.10331
434A -> 446A -0.11207
435A -> 445A -0.12350
436A -> 442A 0.14912
436A -> 446A -0.20313
436A -> 448A 0.12969
436A -> 449A -0.11503
406B -> 437B 0.10701
408B -> 437B 0.17888
431B -> 442B -0.10516
432B -> 439B 0.10086
433B -> 448B -0.10331
434B -> 446B 0.11207
435B -> 445B 0.12350
436B -> 442B -0.14912
436B -> 446B 0.20313
436B -> 448B -0.12969
436B -> 449B 0.11503

Excited State 173: 1.000-A 2.9242 eV 424.00 nm f=0.0044 <S**2>=0.000
395A -> 437A -0.12424
400A -> 437A -0.20336
401A -> 437A -0.29332
402A -> 437A 0.26485
406A -> 437A 0.28801
408A -> 437A 0.36038
395B -> 437B -0.12424
400B -> 437B -0.20336
401B -> 437B -0.29332

402B -> 437B 0.26485
406B -> 437B 0.28801
408B -> 437B 0.36038

Excited State 174: 3.000-A 2.9264 eV 423.67 nm f=0.0000 <S**2>=2.000
398A -> 438A -0.21817
405A -> 438A -0.11401
406A -> 438A -0.39732
407A -> 438A -0.14818
409A -> 438A 0.43671
398B -> 438B 0.21817
405B -> 438B 0.11401
406B -> 438B 0.39732
407B -> 438B 0.14818
409B -> 438B -0.43671

Excited State 175: 1.000-A 2.9416 eV 421.49 nm f=0.0205 <S**2>=0.000
397A -> 438A 0.15935
398A -> 438A -0.17251
399A -> 438A 0.34305
400A -> 438A -0.24781
401A -> 438A 0.13708
403A -> 438A -0.15596
404A -> 438A 0.11714
406A -> 438A -0.24468
407A -> 438A -0.24677
408A -> 438A -0.10289
435A -> 444A 0.14136
436A -> 444A 0.12587
397B -> 438B 0.15935
398B -> 438B -0.17251
399B -> 438B 0.34305
400B -> 438B -0.24781
401B -> 438B 0.13708
403B -> 438B -0.15596
404B -> 438B 0.11714

406B -> 438B -0.24468
407B -> 438B -0.24677
408B -> 438B -0.10289
435B -> 444B 0.14136
436B -> 444B 0.12587

Excited State 176: 3.000-A 2.9576 eV 419.21 nm f=0.0000 <S**2>=2.000
391A -> 438A -0.10102
394A -> 438A -0.10864
397A -> 438A -0.11433
398A -> 438A 0.20967
399A -> 438A 0.30507
402A -> 438A -0.28485
403A -> 438A -0.23374
404A -> 438A 0.10985
405A -> 438A 0.15597
406A -> 438A -0.16176
407A -> 438A -0.21841
408A -> 438A -0.15792
412A -> 438A 0.10292
391B -> 438B 0.10102
394B -> 438B 0.10864
397B -> 438B 0.11433
398B -> 438B -0.20967
399B -> 438B -0.30507
402B -> 438B 0.28485
403B -> 438B 0.23374
404B -> 438B -0.10985
405B -> 438B -0.15597
406B -> 438B 0.16176
407B -> 438B 0.21841
408B -> 438B 0.15792
412B -> 438B -0.10292

Excited State 177: 1.000-A 2.9593 eV 418.96 nm f=0.0113 <S**2>=0.000
431A -> 439A -0.10052

436A -> 442A 0.60757
436A -> 443A -0.20041
431B -> 439B -0.10052
436B -> 442B 0.60757
436B -> 443B -0.20041

Excited State 178: 1.000-A 2.9647 eV 418.21 nm f=0.0061 <S**2>=0.000
397A -> 438A 0.36857
398A -> 438A 0.16539
399A -> 438A -0.10014
401A -> 438A 0.13484
403A -> 438A -0.21314
404A -> 438A -0.11512
405A -> 438A 0.14144
407A -> 438A 0.31095
409A -> 438A -0.23979
397B -> 438B 0.36857
398B -> 438B 0.16539
399B -> 438B -0.10014
401B -> 438B 0.13484
403B -> 438B -0.21314
404B -> 438B -0.11512
405B -> 438B 0.14144
407B -> 438B 0.31095
409B -> 438B -0.23979

Excited State 179: 3.000-A 2.9661 eV 418.00 nm f=0.0000 <S**2>=2.000
392A -> 439A -0.20362
431A -> 439A 0.58894
432A -> 439A -0.13147
433A -> 439A 0.17511
434A -> 439A 0.10613
392B -> 439B 0.20362
431B -> 439B -0.58894
432B -> 439B 0.13147
433B -> 439B -0.17511

434B -> 439B -0.10613

Excited State 180: 1.000-A 2.9732 eV 417.00 nm f=0.0002 <S**2>=0.000
431A -> 439A 0.65179
433A -> 439A 0.18496
434A -> 439A 0.10767
436A -> 442A 0.10053
431B -> 439B 0.65179
433B -> 439B 0.18496
434B -> 439B 0.10767
436B -> 442B 0.10053

Excited State 181: 3.000-A 2.9827 eV 415.68 nm f=0.0000 <S**2>=2.000
393A -> 440A -0.15775
430A -> 440A 0.61962
432A -> 440A 0.10983
433A -> 440A -0.13610
434A -> 440A 0.13620
393B -> 440B 0.15775
430B -> 440B -0.61962
432B -> 440B -0.10983
433B -> 440B 0.13610
434B -> 440B -0.13620

Excited State 182: 1.000-A 2.9876 eV 415.00 nm f=0.0130 <S**2>=0.000
395A -> 437A -0.11749
403A -> 438A 0.10140
404A -> 438A -0.10799
405A -> 438A -0.14546
430A -> 440A 0.42549
435A -> 441A 0.22355
435A -> 442A -0.15083
436A -> 441A 0.24110
436A -> 443A -0.15733
436A -> 444A 0.11732
395B -> 437B -0.11749

403B -> 438B 0.10140
404B -> 438B -0.10799
405B -> 438B -0.14546
430B -> 440B 0.42549
435B -> 441B 0.22355
435B -> 442B -0.15083
436B -> 441B 0.24110
436B -> 443B -0.15733
436B -> 444B 0.11732

Excited State 183: 1.000-A 2.9900 eV 414.66 nm f=0.0001 <S**2>=0.000
397A -> 438A -0.11461
398A -> 438A 0.21172
401A -> 438A -0.17871
402A -> 438A -0.15980
403A -> 438A -0.30496
404A -> 438A 0.18544
405A -> 438A 0.31082
407A -> 438A -0.14231
430A -> 440A 0.25779
397B -> 438B -0.11461
398B -> 438B 0.21172
401B -> 438B -0.17871
402B -> 438B -0.15980
403B -> 438B -0.30496
404B -> 438B 0.18544
405B -> 438B 0.31082
407B -> 438B -0.14231
430B -> 440B 0.25779

Excited State 184: 1.000-A 2.9949 eV 413.98 nm f=0.0129 <S**2>=0.000
395A -> 437A 0.12972
430A -> 440A 0.44361
435A -> 441A -0.23714
435A -> 442A 0.16375
436A -> 441A -0.28566

436A -> 442A 0.12724
436A -> 443A 0.19272
395B -> 437B 0.12972
430B -> 440B 0.44361
435B -> 441B -0.23714
435B -> 442B 0.16375
436B -> 441B -0.28566
436B -> 442B 0.12724
436B -> 443B 0.19272

Excited State 185: 3.000-A 2.9959 eV 413.85 nm f=0.0000 <S**2>=2.000
399A -> 438A 0.17655
401A -> 438A 0.25494
402A -> 438A -0.25342
403A -> 438A 0.25973
405A -> 438A 0.17042
407A -> 438A 0.45445
408A -> 438A -0.14638
399B -> 438B -0.17655
401B -> 438B -0.25494
402B -> 438B 0.25342
403B -> 438B -0.25973
405B -> 438B -0.17042
407B -> 438B -0.45445
408B -> 438B 0.14638

Excited State 186: 3.000-A 2.9970 eV 413.70 nm f=0.0000 <S**2>=2.000
399A -> 438A -0.14112
402A -> 438A 0.10135
403A -> 438A 0.17090
404A -> 438A 0.51717
405A -> 438A 0.37993
399B -> 438B 0.14112
402B -> 438B -0.10135
403B -> 438B -0.17090
404B -> 438B -0.51717

405B -> 438B -0.37993

Excited State 187: 1.000-A 2.9999 eV 413.30 nm f=0.0003 <S**2>=0.000
401A -> 438A 0.15834
403A -> 438A 0.34048
404A -> 438A 0.39412
405A -> 438A 0.34249
407A -> 438A 0.23485
401B -> 438B 0.15834
403B -> 438B 0.34048
404B -> 438B 0.39412
405B -> 438B 0.34249
407B -> 438B 0.23485

Excited State 188: 1.000-A 3.0071 eV 412.31 nm f=0.0006 <S**2>=0.000
397A -> 438A -0.24325
399A -> 438A 0.34806
401A -> 438A 0.13214
402A -> 438A -0.34220
404A -> 438A -0.27758
407A -> 438A 0.27116
408A -> 438A -0.12236
397B -> 438B -0.24325
399B -> 438B 0.34806
401B -> 438B 0.13214
402B -> 438B -0.34220
404B -> 438B -0.27758
407B -> 438B 0.27116
408B -> 438B -0.12236

Excited State 189: 3.000-A 3.0099 eV 411.92 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.36096
399A -> 437A -0.17969
402A -> 437A 0.43586
403A -> 437A 0.11044
404A -> 437A -0.18603

405A -> 437A 0.19481
398B -> 437B 0.36096
399B -> 437B 0.17969
402B -> 437B -0.43586
403B -> 437B -0.11044
404B -> 437B 0.18603
405B -> 437B -0.19481

Excited State 190: 3.000-A 3.0248 eV 409.90 nm f=0.0000 <S**2>=2.000
435A -> 442A -0.14346
435A -> 443A -0.11016
436A -> 441A -0.39806
436A -> 442A 0.37631
436A -> 443A 0.25600
436A -> 444A -0.12278
435B -> 442B 0.14346
435B -> 443B 0.11016
436B -> 441B 0.39806
436B -> 442B -0.37631
436B -> 443B -0.25600
436B -> 444B 0.12278

Excited State 191: 3.000-A 3.0304 eV 409.13 nm f=0.0000 <S**2>=2.000
399A -> 437A -0.13279
431A -> 441A 0.13880
433A -> 441A 0.15676
433A -> 443A 0.17945
434A -> 441A 0.17876
434A -> 443A 0.24295
435A -> 441A 0.18342
435A -> 442A 0.13130
436A -> 441A 0.18981
436A -> 442A 0.18322
436A -> 448A 0.13568
399B -> 437B 0.13279
431B -> 441B -0.13880

433B -> 441B -0.15676
433B -> 443B -0.17945
434B -> 441B -0.17876
434B -> 443B -0.24295
435B -> 441B -0.18342
435B -> 442B -0.13130
436B -> 441B -0.18981
436B -> 442B -0.18322
436B -> 448B -0.13568

Excited State 192: 1.000-A 3.0310 eV 409.05 nm f=0.0007 <S**2>=0.000
398A -> 437A 0.42752
399A -> 437A 0.33810
402A -> 437A -0.34805
404A -> 437A 0.13782
405A -> 437A -0.14871
398B -> 437B 0.42752
399B -> 437B 0.33810
402B -> 437B -0.34805
404B -> 437B 0.13782
405B -> 437B -0.14871

Excited State 193: 3.000-A 3.0380 eV 408.11 nm f=0.0000 <S**2>=2.000
398A -> 438A 0.28352
400A -> 438A -0.35010
403A -> 438A 0.42643
405A -> 438A -0.19583
407A -> 438A -0.15888
398B -> 438B -0.28352
400B -> 438B 0.35010
403B -> 438B -0.42643
405B -> 438B 0.19583
407B -> 438B 0.15888

Excited State 194: 1.000-A 3.0436 eV 407.37 nm f=0.0000 <S**2>=0.000
415A -> 440A 0.46655

416A -> 440A 0.45116
417A -> 440A -0.11436
418A -> 440A -0.13843
429A -> 440A 0.10135
415B -> 440B 0.46655
416B -> 440B 0.45116
417B -> 440B -0.11436
418B -> 440B -0.13843
429B -> 440B 0.10135

Excited State 195: 1.000-A 3.0468 eV 406.93 nm f=0.0000 <S**2>=0.000
410A -> 439A 0.13211
413A -> 439A 0.19343
414A -> 439A 0.62151
415A -> 439A 0.12009
416A -> 439A -0.12750
410B -> 439B 0.13211
413B -> 439B 0.19343
414B -> 439B 0.62151
415B -> 439B 0.12009
416B -> 439B -0.12750

Excited State 196: 1.000-A 3.0553 eV 405.81 nm f=0.0012 <S**2>=0.000
398A -> 438A -0.37547
400A -> 438A 0.43038
401A -> 438A 0.12797
402A -> 438A 0.13735
403A -> 438A -0.27772
407A -> 438A 0.13234
398B -> 438B -0.37547
400B -> 438B 0.43038
401B -> 438B 0.12797
402B -> 438B 0.13735
403B -> 438B -0.27772
407B -> 438B 0.13234

Excited State 197: 1.000-A 3.0576 eV 405.49 nm f=0.0091 <S**2>=0.000

| | |
|---|---|
| 395A -> 437A | -0.11437 |
| 435A -> 441A | -0.35411 |
| 435A -> 442A | 0.38765 |
| 435A -> 443A | 0.11020 |
| 436A -> 441A | 0.24168 |
| 436A -> 442A | -0.16751 |
| 436A -> 443A | -0.27394 |
| 395B -> 437B | -0.11437 |
| 435B -> 441B | -0.35411 |
| 435B -> 442B | 0.38765 |
| 435B -> 443B | 0.11020 |
| 436B -> 441B | 0.24168 |
| 436B -> 442B | -0.16751 |
| 436B -> 443B | -0.27394 |

Excited State 198: 3.000-A 3.0622 eV 404.89 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 396A -> 437A | 0.16973 |
| 398A -> 437A | -0.27809 |
| 399A -> 437A | 0.47125 |
| 435A -> 441A | 0.12942 |
| 435A -> 442A | 0.20975 |
| 436A -> 441A | 0.10003 |
| 436A -> 442A | 0.13056 |
| 396B -> 437B | -0.16973 |
| 398B -> 437B | 0.27809 |
| 399B -> 437B | -0.47125 |
| 435B -> 441B | -0.12942 |
| 435B -> 442B | -0.20975 |
| 436B -> 441B | -0.10003 |
| 436B -> 442B | -0.13056 |

Excited State 199: 3.000-A 3.0659 eV 404.40 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 398A -> 437A | -0.21625 |
| 399A -> 437A | 0.27433 |
| 435A -> 441A | -0.16125 |

| | |
|---|---|
| 435A -> 442A | -0.29636 |
| 435A -> 443A | 0.17573 |
| 435A -> 447A | -0.11146 |
| 436A -> 442A | -0.17529 |
| 436A -> 443A | 0.13043 |
| 436A -> 448A | 0.11336 |
| 398B -> 437B | 0.21625 |
| 399B -> 437B | -0.27433 |
| 435B -> 441B | 0.16125 |
| 435B -> 442B | 0.29636 |
| 435B -> 443B | -0.17573 |
| 435B -> 447B | 0.11146 |
| 436B -> 442B | 0.17529 |
| 436B -> 443B | -0.13043 |
| 436B -> 448B | -0.11336 |

Excited State 200: 1.000-A 3.0705 eV 403.79 nm f=0.0034 <S**2>=0.000

| | |
|---|---|
| 396A -> 437A | 0.12369 |
| 398A -> 437A | -0.42557 |
| 399A -> 437A | 0.51611 |
| 411A -> 437A | -0.10239 |
| 396B -> 437B | 0.12369 |
| 398B -> 437B | -0.42557 |
| 399B -> 437B | 0.51611 |
| 411B -> 437B | -0.10239 |

**Table S12.** Standard orientation of the optimized geometry for the open-ring isomer (OF5) of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | -0.080562 | -2.403347 | 0.080187 |
| N | 4.165477 | -3.581871 | 0.047636 |
| C | 3.172356 | -2.821134 | 0.663452 |
| C | 3.480636 | -2.187521 | 1.910945 |
| C | 4.861924 | -1.874248 | 2.237732 |
| C | 5.890941 | -1.702504 | 1.248314 |
| C | 5.612086 | -1.191721 | -0.071472 |
| C | 6.60822 | -0.946124 | -0.96958 |
| C | 8.009099 | -1.15425 | -0.63746 |
| C | 8.282241 | -1.707211 | 0.690143 |
| C | 7.276247 | -1.937422 | 1.58361 |
| O | 8.945545 | -0.834881 | -1.434239 |
| C | 2.502116 | -2.072476 | 2.934083 |
| C | 2.854306 | -1.778631 | 4.236228 |
| C | 4.210542 | -1.570622 | 4.581536 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 5.185155 | -1.630217 | 3.607897 | Cl | 0.404413 | -0.179703 | 1.584913 |
| C | 3.599039 | -4.220789 | -0.984426 | Cl | 0.120836 | -0.336259 | -1.633429 |
| C | 2.200912 | -3.840358 | -1.048451 | Ir | 0.212394 | 1.906814 | -0.080021 |
| N | 1.952553 | -2.978957 | 0.001199 | N | -4.36379 | -2.026104 | 0.067715 |
| C | 4.386001 | -5.187399 | -1.764851 | C | -3.17892 | -1.788463 | -0.604419 |
| C | 1.082648 | -4.235942 | -1.846333 | C | -3.500457 | -1.440756 | -1.988706 |
| C | 1.159847 | -5.013917 | -3.027646 | C | -4.911471 | -1.479067 | -2.11079 |
| C | -0.000755 | -5.455025 | -3.646705 | C | -5.586941 | -1.786599 | -0.753265 |
| C | -1.253126 | -5.134703 | -3.087105 | C | -6.439936 | -3.032528 | -0.842933 |
| C | -1.344178 | -4.322237 | -1.956124 | C | -7.774303 | -3.010144 | -0.686774 |
| C | -0.190036 | -3.800241 | -1.336855 | C | -8.500359 | -1.772599 | -0.336561 |
| C | 5.706655 | -4.85259 | -2.128622 | C | -7.687105 | -0.556187 | -0.152014 |
| C | 6.507637 | -5.765923 | -2.81697 | C | -6.350087 | -0.555651 | -0.300691 |
| C | 6.010524 | -7.034314 | -3.142113 | O | -9.745005 | -1.761437 | -0.196317 |
| C | 4.708164 | -7.385867 | -2.766693 | C | -2.718033 | -1.211278 | -3.125671 |
| C | 3.901388 | -6.472383 | -2.082872 | C | -3.358817 | -1.007559 | -4.354874 |
| N | 4.579633 | 2.165567 | 0.436823 | C | -4.754942 | -1.038147 | -4.463414 |
| C | 3.535875 | 1.904878 | -0.444751 | C | -5.545585 | -1.275993 | -3.329039 |
| C | 3.8659 | 1.617652 | -1.815741 | C | -4.104362 | -2.669555 | 1.278442 |
| C | 5.179081 | 1.990251 | -2.291733 | C | -2.717706 | -2.779556 | 1.330942 |
| C | 6.00473 | 2.980281 | -1.636367 | N | -2.156616 | -2.199936 | 0.168204 |
| C | 5.454797 | 4.238596 | -1.183496 | C | -5.174714 | -3.186032 | 2.155997 |
| C | 6.253093 | 5.24335 | -0.72754 | C | -1.784561 | -3.513252 | 2.173057 |
| C | 7.702596 | 5.079537 | -0.639156 | C | -2.124419 | -4.148873 | 3.380364 |
| C | 8.246057 | 3.797955 | -1.102163 | C | -1.207124 | -4.991652 | 4.011702 |
| C | 7.43891 | 2.819582 | -1.604452 | C | 0.044597 | -5.216502 | 3.425867 |
| O | 8.457606 | 5.996026 | -0.203013 | C | 0.403919 | -4.551737 | 2.246008 |
| C | 3.018686 | 0.891646 | -2.684323 | C | -0.474203 | -3.647751 | 1.62215 |
| C | 3.474946 | 0.435679 | -3.910118 | C | -6.100047 | -2.319528 | 2.766509 |
| C | 4.801143 | 0.69032 | -4.325605 | C | -7.137187 | -2.830732 | 3.553309 |
| C | 5.639509 | 1.442994 | -3.521896 | C | -7.259115 | -4.210836 | 3.749795 |
| C | 4.045742 | 2.665309 | 1.563871 | C | -6.336969 | -5.081082 | 3.155113 |
| C | 2.608842 | 2.664627 | 1.416969 | C | -5.305238 | -4.574788 | 2.360654 |
| N | 2.309648 | 2.103549 | 0.182309 | N | -4.179396 | 2.202514 | -0.58838 |
| C | 4.923733 | 3.05822 | 2.68088 | C | -3.129958 | 1.899549 | 0.278865 |
| C | 1.507949 | 3.207744 | 2.157541 | C | -3.452779 | 1.58855 | 1.647005 |
| C | 1.587852 | 3.81059 | 3.434622 | C | -2.630391 | 0.767949 | 2.451439 |
| C | 0.492186 | 4.488451 | 3.954117 | C | -3.062681 | 0.304916 | 3.682475 |
| C | -0.691628 | 4.588617 | 3.199266 | C | -4.344975 | 0.647323 | 4.165954 |
| C | -0.801413 | 3.945744 | 1.964887 | C | -5.156549 | 1.489201 | 3.425957 |
| C | 0.262824 | 3.190859 | 1.44255 | C | -3.639394 | 2.707051 | -1.710872 |
| C | 5.964325 | 2.192077 | 3.07029 | C | -2.199328 | 2.656732 | -1.57982 |
| C | 6.856866 | 2.560721 | 4.078897 | N | -1.903188 | 2.077951 | -0.351803 |
| C | 6.73607 | 3.806024 | 4.708238 | C | -4.506353 | 3.220561 | -2.78639 |
| C | 5.721563 | 4.684881 | 4.312507 | C | -1.101068 | 3.175027 | -2.334392 |
| C | 4.824323 | 4.316978 | 3.305309 | C | -1.187435 | 3.755218 | -3.624325 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.092192 | 4.413414 | -4.163574 | H | -5.910764 | -3.949486 | -1.084971 |
| C | 1.099555 | 4.519107 | -3.417018 | H | -8.376256 | -3.906266 | -0.790703 |
| C | 1.217012 | 3.897695 | -2.17476 | H | -8.226712 | 0.346885 | 0.11322 |
| C | 0.152149 | 3.153966 | -1.627875 | H | -5.759227 | 0.35068 | -0.188033 |
| C | -5.621604 | 2.468715 | -3.202978 | H | -1.641932 | -1.17884 | -3.052727 |
| C | -6.501914 | 2.971987 | -4.163202 | H | -2.755561 | -0.827202 | -5.238145 |
| C | -6.294761 | 4.242428 | -4.714237 | H | -5.228419 | -0.882633 | -5.42684 |
| C | -5.203351 | 5.009448 | -4.29072 | H | -6.627399 | -1.31664 | -3.404429 |
| C | -4.317558 | 4.50567 | -3.334224 | H | -3.105288 | -3.999608 | 3.816551 |
| H | 4.589461 | -0.947789 | -0.32501 | H | -1.474494 | -5.483378 | 4.94165 |
| H | 6.391601 | -0.531399 | -1.944883 | H | 0.747949 | -5.900958 | 3.89123 |
| H | 9.317854 | -1.920948 | 0.931171 | H | 1.385025 | -4.728816 | 1.821781 |
| H | 7.510892 | -2.368965 | 2.550074 | H | -6.000875 | -1.249497 | 2.628938 |
| H | 1.476059 | -2.292772 | 2.698202 | H | -7.847758 | -2.151814 | 4.013631 |
| H | 2.086259 | -1.731814 | 5.000218 | H | -8.064916 | -4.605075 | 4.360373 |
| H | 4.480659 | -1.339922 | 5.60659 | H | -6.425926 | -6.152555 | 3.302604 |
| H | 6.210075 | -1.399546 | 3.870905 | H | -4.59483 | -5.250075 | 1.895385 |
| H | 2.125933 | -5.262257 | -3.448289 | H | -1.671841 | 0.450065 | 2.073276 |
| H | 0.056304 | -6.05071 | -4.551677 | H | -2.418277 | -0.349959 | 4.25862 |
| H | -2.160598 | -5.508801 | -3.552683 | H | -4.681657 | 0.276493 | 5.128372 |
| H | -2.322972 | -4.078458 | -1.565686 | H | -6.103361 | 1.819469 | 3.838372 |
| H | 6.087582 | -3.871637 | -1.867752 | H | -2.10662 | 3.681561 | -4.190476 |
| H | 7.51837 | -5.488507 | -3.098559 | H | -0.155706 | 4.855802 | -5.152145 |
| H | 6.633923 | -7.744108 | -3.676578 | H | 1.941054 | 5.072064 | -3.824229 |
| H | 4.324 | -8.374903 | -2.995635 | H | 2.150819 | 3.963779 | -1.633168 |
| H | 2.904775 | -6.763729 | -1.770278 | H | -5.786502 | 1.490354 | -2.769662 |
| H | 4.384113 | 4.387044 | -1.263011 | H | -7.352859 | 2.375894 | -4.477619 |
| H | 5.84818 | 6.202768 | -0.426604 | H | -6.982893 | 4.635447 | -5.455612 |
| H | 9.31884 | 3.663417 | -1.019641 | H | -5.049714 | 6.005974 | -4.692047 |
| H | 7.865277 | 1.871721 | -1.918173 | H | -3.495188 | 5.121822 | -2.988442 |
| H | 2.028313 | 0.623363 | -2.354408 | C | -4.714408 | 2.045971 | 2.191438 |
| H | 2.811248 | -0.148318 | -4.538662 | C | -5.481911 | 3.134898 | 1.625849 |
| H | 5.154521 | 0.319359 | -5.281761 | C | -6.920357 | 3.131213 | 1.720212 |
| H | 6.635831 | 1.696387 | -3.866381 | C | -4.855007 | 4.327808 | 1.111553 |
| H | 2.501241 | 3.740245 | 4.010175 | C | -7.669751 | 4.181978 | 1.274607 |
| H | 0.553839 | 4.949746 | 4.934172 | H | -7.410366 | 2.241105 | 2.101105 |
| H | -1.533302 | 5.153997 | 3.588754 | C | -5.585182 | 5.406122 | 0.706262 |
| H | -1.72864 | 4.007505 | 1.412496 | H | -3.773306 | 4.373992 | 1.097924 |
| H | 6.064055 | 1.237214 | 2.567867 | H | -8.753831 | 4.159867 | 1.294943 |
| H | 7.651545 | 1.880682 | 4.369507 | H | -5.109733 | 6.315888 | 0.357993 |
| H | 7.433413 | 4.093863 | 5.488379 | C | -7.044105 | 5.394223 | 0.740221 |
| H | 5.63809 | 5.663323 | 4.774675 | O | -7.738963 | 6.378863 | 0.350997 |
| H | 4.066063 | 5.020376 | 2.97955 | | | | |

Excited State 1: 3.000-A -0.5846 eV -2120.87 nm f=-0.0000 <S**2>=2.000

431A -> 437A -0.17750
434A -> 437A 0.39989
434A -> 438A -0.19832
435A -> 437A 0.47986
436A -> 437A 0.18638
431B -> 437B 0.17750
434B -> 437B -0.39989
434B -> 438B 0.19832
435B -> 437B -0.47986
436B -> 437B -0.18638
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -6023.94357822
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.000-A -0.5782 eV -2144.49 nm f=-0.0000 <S**2>=2.000
433A -> 439A -0.33505
435A -> 439A 0.23198
436A -> 439A -0.56531
433B -> 439B 0.33505
435B -> 439B -0.23198
436B -> 439B 0.56531

Excited State 3: 3.000-A -0.5675 eV -2184.84 nm f=-0.0000 <S**2>=2.000
431A -> 438A 0.11311
434A -> 437A 0.23894
434A -> 438A 0.34570
435A -> 438A -0.47825
436A -> 438A -0.23708
431B -> 438B -0.11311
434B -> 437B -0.23894
434B -> 438B -0.34570
435B -> 438B 0.47825
436B -> 438B 0.23708

Excited State 4: 3.000-A 0.5273 eV 2351.37 nm f=0.0000 <S**2>=2.000
431A -> 437A 0.12821

434A -> 437A -0.16301
436A -> 437A 0.65544
431B -> 437B -0.12821
434B -> 437B 0.16301
436B -> 437B -0.65544

Excited State 5: 1.000-A 0.5497 eV 2255.36 nm f=0.0025 <S**2>=0.000
435A -> 437A -0.18838
436A -> 437A 0.67338
435B -> 437B -0.18838
436B -> 437B 0.67338

Excited State 6: 3.000-A 0.6141 eV 2018.80 nm f=0.0000 <S**2>=2.000
431A -> 437A 0.17241
431A -> 438A -0.11855
434A -> 437A -0.32404
435A -> 437A 0.38063
436A -> 437A -0.12482
436A -> 438A -0.43164
431B -> 437B -0.17241
431B -> 438B 0.11855
434B -> 437B 0.32404
435B -> 437B -0.38063
436B -> 437B 0.12482
436B -> 438B 0.43164

Excited State 7: 1.000-A 0.6577 eV 1885.01 nm f=0.0035 <S**2>=0.000
435A -> 438A -0.18378
436A -> 438A 0.65990
435B -> 438B -0.18378
436B -> 438B 0.65990

Excited State 8: 3.000-A 0.6677 eV 1856.86 nm f=0.0000 <S**2>=2.000
431A -> 437A -0.12582
434A -> 437A 0.21026
434A -> 438A -0.10343

435A -> 437A -0.27660
435A -> 438A 0.31367
436A -> 438A -0.48647
431B -> 437B 0.12582
434B -> 437B -0.21026
434B -> 438B 0.10343
435B -> 437B 0.27660
435B -> 438B -0.31367
436B -> 438B 0.48647

Excited State 9: 1.000-A 0.7271 eV 1705.08 nm f=0.0433 <S**2>=0.000
434A -> 437A -0.30367
435A -> 437A 0.58261
435A -> 438A -0.18118
436A -> 437A 0.14585
434B -> 437B -0.30367
435B -> 437B 0.58261
435B -> 438B -0.18118
436B -> 437B 0.14585

Excited State 10: 3.000-A 0.7540 eV 1644.39 nm f=0.0000 <S**2>=2.000
430A -> 439A 0.14707
433A -> 439A -0.47890
435A -> 439A 0.25984
436A -> 439A 0.41107
430B -> 439B -0.14707
433B -> 439B 0.47890
435B -> 439B -0.25984
436B -> 439B -0.41107

Excited State 11: 1.000-A 0.7844 eV 1580.68 nm f=0.0017 <S**2>=0.000
434A -> 439A -0.12293
435A -> 438A 0.13458
435A -> 439A 0.54334
436A -> 439A 0.40519
434B -> 439B -0.12293

435B -> 438B 0.13458
435B -> 439B 0.54334
436B -> 439B 0.40519

Excited State 12: 3.000-A 0.8058 eV 1538.73 nm f=0.0000 <S**2>=2.000
431A -> 438A 0.13720
433A -> 439A -0.24826
434A -> 438A 0.34250
435A -> 437A 0.14490
435A -> 438A 0.23395
435A -> 439A -0.44689
431B -> 438B -0.13720
433B -> 439B 0.24826
434B -> 438B -0.34250
435B -> 437B -0.14490
435B -> 438B -0.23395
435B -> 439B 0.44689

Excited State 13: 3.000-A 0.8082 eV 1534.15 nm f=0.0000 <S**2>=2.000
431A -> 438A -0.14260
433A -> 439A -0.23801
434A -> 438A -0.35150
435A -> 437A -0.14136
435A -> 438A -0.30687
435A -> 439A -0.39431
431B -> 438B 0.14260
433B -> 439B 0.23801
434B -> 438B 0.35150
435B -> 437B 0.14136
435B -> 438B 0.30687
435B -> 439B 0.39431

Excited State 14: 1.000-A 0.8487 eV 1460.81 nm f=0.0262 <S**2>=0.000
433A -> 439A -0.10225
434A -> 437A 0.19823
434A -> 438A 0.24564

435A -> 437A 0.18778
435A -> 438A 0.49088
435A -> 439A -0.24085
436A -> 438A 0.16261
433B -> 439B -0.10225
434B -> 437B 0.19823
434B -> 438B 0.24564
435B -> 437B 0.18778
435B -> 438B 0.49088
435B -> 439B -0.24085
436B -> 438B 0.16261

Excited State 15: 1.000-A 0.9050 eV 1370.05 nm f=0.0882 <S**2>=0.000
433A -> 439A 0.42022
434A -> 438A 0.11527
435A -> 437A 0.11569
435A -> 438A 0.16708
435A -> 439A 0.28954
436A -> 439A -0.41171
433B -> 439B 0.42022
434B -> 438B 0.11527
435B -> 437B 0.11569
435B -> 438B 0.16708
435B -> 439B 0.28954
436B -> 439B -0.41171

Excited State 16: 3.000-A 0.9116 eV 1360.04 nm f=0.0000 <S**2>=2.000
431A -> 437A -0.12717
432A -> 437A 0.16566
433A -> 437A 0.64009
431B -> 437B 0.12717
432B -> 437B -0.16566
433B -> 437B -0.64009

Excited State 17: 1.000-A 0.9281 eV 1335.95 nm f=0.0001 <S**2>=0.000
433A -> 437A 0.68490

433B -> 437B 0.68490

Excited State 18: 3.000-A 1.0057 eV 1232.85 nm f=0.0000 <S**2>=2.000

429A -> 437A -0.26626
429A -> 438A 0.11929
431A -> 437A -0.32226
432A -> 437A 0.36582
432A -> 438A -0.14522
433A -> 437A -0.26193
433A -> 438A -0.14036
434A -> 437A -0.17335
429B -> 437B 0.26626
429B -> 438B -0.11929
431B -> 437B 0.32226
432B -> 437B -0.36582
432B -> 438B 0.14522
433B -> 437B 0.26193
433B -> 438B 0.14036
434B -> 437B 0.17335

Excited State 19: 1.000-A 1.0633 eV 1166.03 nm f=0.0218 <S**2>=0.000

429A -> 437A 0.12972
431A -> 437A 0.13293
432A -> 437A -0.25542
432A -> 438A 0.13621
433A -> 438A 0.52287
434A -> 437A 0.23614
434A -> 438A -0.12918
435A -> 437A 0.15136
429B -> 437B 0.12972
431B -> 437B 0.13293
432B -> 437B -0.25542
432B -> 438B 0.13621
433B -> 438B 0.52287
434B -> 437B 0.23614
434B -> 438B -0.12918

435B -> 437B 0.15136

Excited State 20: 3.000-A 1.0675 eV 1161.43 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.10341
432A -> 437A -0.15455
433A -> 438A -0.66019
429B -> 437B -0.10341
432B -> 437B 0.15455
433B -> 438B 0.66019

Excited State 21: 1.000-A 1.0739 eV 1154.57 nm f=0.0226 <S**2>=0.000
429A -> 437A -0.14190
431A -> 437A -0.17390
432A -> 437A 0.27559
433A -> 438A 0.45178
434A -> 437A -0.26955
434A -> 438A 0.23300
435A -> 437A -0.12062
435A -> 438A 0.11695
429B -> 437B -0.14190
431B -> 437B -0.17390
432B -> 437B 0.27559
433B -> 438B 0.45178
434B -> 437B -0.26955
434B -> 438B 0.23300
435B -> 437B -0.12062
435B -> 438B 0.11695

Excited State 22: 3.000-A 1.0814 eV 1146.47 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.19500
432A -> 439A -0.54364
434A -> 439A 0.35457
435A -> 439A 0.10964
429B -> 439B 0.19500
432B -> 439B 0.54364
434B -> 439B -0.35457

435B -> 439B -0.10964

Excited State 23: 3.000-A 1.0939 eV 1133.47 nm f=0.0000 <S**2>=2.000
429A -> 437A -0.20409
431A -> 437A 0.47024
431A -> 438A -0.13392
432A -> 437A 0.31348
432A -> 438A -0.11315
434A -> 437A 0.24145
429B -> 437B 0.20409
431B -> 437B -0.47024
431B -> 438B 0.13392
432B -> 437B -0.31348
432B -> 438B 0.11315
434B -> 437B -0.24145

Excited State 24: 1.000-A 1.1082 eV 1118.76 nm f=0.0011 <S**2>=0.000
434A -> 439A 0.67133
435A -> 439A 0.15767
434B -> 439B 0.67133
435B -> 439B 0.15767

Excited State 25: 3.000-A 1.1206 eV 1106.41 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.13327
431A -> 439A -0.11036
432A -> 439A -0.33001
434A -> 439A -0.58525
429B -> 439B 0.13327
431B -> 439B 0.11036
432B -> 439B 0.33001
434B -> 439B 0.58525

Excited State 26: 1.000-A 1.1407 eV 1086.95 nm f=0.0292 <S**2>=0.000
429A -> 437A -0.16392
431A -> 437A 0.25725
432A -> 437A 0.47122

434A -> 437A 0.11894
434A -> 438A -0.36458
429B -> 437B -0.16392
431B -> 437B 0.25725
432B -> 437B 0.47122
434B -> 437B 0.11894
434B -> 438B -0.36458

Excited State 27: 3.000-A 1.1432 eV 1084.56 nm f=0.0000 <S**2>=2.000
429A -> 438A 0.38862
432A -> 437A -0.21042
432A -> 438A -0.48548
433A -> 438A 0.10596
434A -> 438A 0.12943
429B -> 438B -0.38862
432B -> 437B 0.21042
432B -> 438B 0.48548
433B -> 438B -0.10596
434B -> 438B -0.12943

Excited State 28: 3.000-A 1.1510 eV 1077.22 nm f=0.0000 <S**2>=2.000
422A -> 437A 0.66790
422A -> 438A -0.16622
422B -> 437B -0.66790
422B -> 438B 0.16622

Excited State 29: 1.000-A 1.1859 eV 1045.51 nm f=0.0055 <S**2>=0.000
429A -> 438A -0.20575
431A -> 437A -0.21203
432A -> 437A -0.14827
432A -> 438A 0.35234
432A -> 439A 0.11232
433A -> 439A 0.11681
434A -> 437A -0.31898
434A -> 438A -0.24657
435A -> 438A 0.24666

436A -> 438A 0.10779
429B -> 438B -0.20575
431B -> 437B -0.21203
432B -> 437B -0.14827
432B -> 438B 0.35234
432B -> 439B 0.11232
433B -> 439B 0.11681
434B -> 437B -0.31898
434B -> 438B -0.24657
435B -> 438B 0.24666
436B -> 438B 0.10779
435A <- 438A -0.10157
435B <- 438B -0.10157

Excited State 30: 3.000-A 1.1893 eV 1042.52 nm f=0.0000 <S**2>=2.000
423A -> 437A -0.27885
423A -> 438A -0.62199
423B -> 437B 0.27885
423B -> 438B 0.62199

Excited State 31: 1.000-A 1.2515 eV 990.69 nm f=0.0654 <S**2>=0.000
429A -> 439A 0.12943
432A -> 438A -0.12125
432A -> 439A 0.56687
433A -> 439A 0.18291
435A -> 439A -0.11234
436A -> 439A 0.25299
429B -> 439B 0.12943
432B -> 438B -0.12125
432B -> 439B 0.56687
433B -> 439B 0.18291
435B -> 439B -0.11234
436B -> 439B 0.25299

Excited State 32: 3.000-A 1.2758 eV 971.82 nm f=0.0000 <S**2>=2.000
425A -> 439A -0.67201

425A -> 444A 0.10300
426A -> 439A 0.12390
425B -> 439B 0.67201
425B -> 444B -0.10300
426B -> 439B -0.12390

Excited State 33: 3.000-A 1.2850 eV 964.88 nm f=0.0000 <S**2>=2.000
428A -> 437A -0.12137
429A -> 437A 0.44596
430A -> 437A 0.31663
432A -> 437A 0.38924
428B -> 437B 0.12137
429B -> 437B -0.44596
430B -> 437B -0.31663
432B -> 437B -0.38924

Excited State 34: 1.000-A 1.2974 eV 955.67 nm f=0.0040 <S**2>=0.000
429A -> 437A 0.29233
430A -> 437A 0.40331
431A -> 437A -0.24587
431A -> 438A -0.11636
432A -> 437A 0.28082
432A -> 438A 0.14265
434A -> 437A 0.14036
434A -> 438A 0.11481
429B -> 437B 0.29233
430B -> 437B 0.40331
431B -> 437B -0.24587
431B -> 438B -0.11636
432B -> 437B 0.28082
432B -> 438B 0.14265
434B -> 437B 0.14036
434B -> 438B 0.11481

Excited State 35: 3.000-A 1.2990 eV 954.46 nm f=0.0000 <S**2>=2.000
431A -> 437A 0.18164

431A -> 438A 0.60387
434A -> 438A -0.23141
431B -> 437B -0.18164
431B -> 438B -0.60387
434B -> 438B 0.23141

Excited State 36: 3.000-A 1.3426 eV 923.44 nm f=0.0000 <S**2>=2.000
429A -> 437A -0.32884
430A -> 437A 0.59644
432A -> 437A -0.11472
429B -> 437B 0.32884
430B -> 437B -0.59644
432B -> 437B 0.11472

Excited State 37: 1.000-A 1.3511 eV 917.64 nm f=0.0050 <S**2>=0.000
429A -> 437A 0.15552
430A -> 437A 0.31806
431A -> 438A 0.36275
432A -> 438A -0.32126
434A -> 437A -0.17107
434A -> 438A -0.22576
435A -> 438A 0.13945
429B -> 437B 0.15552
430B -> 437B 0.31806
431B -> 438B 0.36275
432B -> 438B -0.32126
434B -> 437B -0.17107
434B -> 438B -0.22576
435B -> 438B 0.13945

Excited State 38: 1.000-A 1.3563 eV 914.13 nm f=0.0007 <S**2>=0.000
429A -> 437A 0.50513
430A -> 437A -0.43810
431A -> 438A 0.11688
432A -> 437A 0.15224
429B -> 437B 0.50513

430B -> 437B -0.43810
431B -> 438B 0.11688
432B -> 437B 0.15224

Excited State 39: 3.000-A 1.4058 eV 881.94 nm f=0.0000 <S**2>=2.000
428A -> 439A -0.42913
429A -> 439A -0.16074
430A -> 439A 0.42077
431A -> 439A -0.26447
433A -> 439A 0.11607
428B -> 439B 0.42913
429B -> 439B 0.16074
430B -> 439B -0.42077
431B -> 439B 0.26447
433B -> 439B -0.11607

Excited State 40: 1.000-A 1.4168 eV 875.09 nm f=0.0813 <S**2>=0.000
428A -> 437A 0.17547
429A -> 437A 0.17101
429A -> 438A 0.14522
430A -> 437A 0.12218
431A -> 437A 0.41159
431A -> 438A 0.10678
432A -> 438A 0.33335
434A -> 437A -0.18595
434A -> 438A 0.19125
435A -> 437A -0.16891
428B -> 437B 0.17547
429B -> 437B 0.17101
429B -> 438B 0.14522
430B -> 437B 0.12218
431B -> 437B 0.41159
431B -> 438B 0.10678
432B -> 438B 0.33335
434B -> 437B -0.18595
434B -> 438B 0.19125

435B -> 437B -0.16891

Excited State 41: 1.000-A 1.4203 eV 872.96 nm f=0.1526 <S**2>=0.000
425A -> 439A -0.11356
430A -> 439A 0.12900
432A -> 439A -0.32025
433A -> 439A 0.48562
435A -> 439A -0.15345
436A -> 439A 0.31367
425B -> 439B -0.11356
430B -> 439B 0.12900
432B -> 439B -0.32025
433B -> 439B 0.48562
435B -> 439B -0.15345
436B -> 439B 0.31367
436A <- 439A -0.15191
436B <- 439B -0.15191

Excited State 42: 1.000-A 1.4362 eV 863.27 nm f=0.0067 <S**2>=0.000
428A -> 437A -0.14637
429A -> 437A -0.15302
429A -> 438A 0.22144
431A -> 437A -0.18932
431A -> 438A 0.46494
432A -> 438A 0.28854
434A -> 437A 0.16462
435A -> 438A -0.13702
428B -> 437B -0.14637
429B -> 437B -0.15302
429B -> 438B 0.22144
431B -> 437B -0.18932
431B -> 438B 0.46494
432B -> 438B 0.28854
434B -> 437B 0.16462
435B -> 438B -0.13702

Excited State 43: 3.000-A 1.4466 eV 857.06 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 427A -> 437A | 0.14509 |
| 428A -> 437A | 0.31700 |
| 429A -> 437A | 0.13832 |
| 429A -> 438A | 0.40892 |
| 430A -> 438A | 0.12409 |
| 432A -> 438A | 0.37981 |
| 427B -> 437B | -0.14509 |
| 428B -> 437B | -0.31700 |
| 429B -> 437B | -0.13832 |
| 429B -> 438B | -0.40892 |
| 430B -> 438B | -0.12409 |
| 432B -> 438B | -0.37981 |

Excited State 44: 3.000-A 1.4541 eV 852.65 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 427A -> 437A | 0.17401 |
| 427A -> 438A | -0.11482 |
| 428A -> 437A | 0.48863 |
| 429A -> 438A | -0.28047 |
| 430A -> 439A | 0.16142 |
| 432A -> 438A | -0.23688 |
| 427B -> 437B | -0.17401 |
| 427B -> 438B | 0.11482 |
| 428B -> 437B | -0.48863 |
| 429B -> 438B | 0.28047 |
| 430B -> 439B | -0.16142 |
| 432B -> 438B | 0.23688 |

Excited State 45: 3.000-A 1.4588 eV 849.88 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 428A -> 437A | 0.16481 |
| 428A -> 439A | -0.27203 |
| 430A -> 439A | -0.48182 |
| 431A -> 439A | -0.28508 |
| 432A -> 439A | 0.17726 |
| 433A -> 439A | -0.12483 |
| 428B -> 437B | -0.16481 |

428B -> 439B 0.27203
430B -> 439B 0.48182
431B -> 439B 0.28508
432B -> 439B -0.17726
433B -> 439B 0.12483

Excited State 46: 1.000-A 1.4748 eV 840.66 nm f=0.0051 <S**2>=0.000
428A -> 439A 0.41982
429A -> 439A 0.16818
430A -> 439A -0.27107
431A -> 439A 0.43841
428B -> 439B 0.41982
429B -> 439B 0.16818
430B -> 439B -0.27107
431B -> 439B 0.43841

Excited State 47: 1.000-A 1.4893 eV 832.52 nm f=0.0138 <S**2>=0.000
422A -> 437A -0.18153
427A -> 437A 0.13272
428A -> 437A 0.60518
431A -> 437A -0.13774
431A -> 438A 0.12049
422B -> 437B -0.18153
427B -> 437B 0.13272
428B -> 437B 0.60518
431B -> 437B -0.13774
431B -> 438B 0.12049

Excited State 48: 1.000-A 1.5330 eV 808.76 nm f=0.0081 <S**2>=0.000
425A -> 439A 0.10849
430A -> 439A 0.60466
431A -> 439A 0.29378
425B -> 439B 0.10849
430B -> 439B 0.60466
431B -> 439B 0.29378

Excited State 49: 1.000-A 1.5340 eV 808.22 nm f=0.0061 <S**2>=0.000

| | |
|---|---|
| 422A -> 437A | 0.58393 |
| 422A -> 438A | -0.14028 |
| 428A -> 437A | 0.11550 |
| 429A -> 438A | -0.15835 |
| 430A -> 438A | -0.22441 |
| 431A -> 438A | 0.10475 |
| 422B -> 437B | 0.58393 |
| 422B -> 438B | -0.14028 |
| 428B -> 437B | 0.11550 |
| 429B -> 438B | -0.15835 |
| 430B -> 438B | -0.22441 |
| 431B -> 438B | 0.10475 |

Excited State 50: 1.000-A 1.5441 eV 802.95 nm f=0.0591 <S**2>=0.000

| | |
|---|---|
| 422A -> 437A | 0.26700 |
| 423A -> 438A | 0.10702 |
| 429A -> 438A | 0.29166 |
| 430A -> 438A | 0.48769 |
| 431A -> 437A | -0.13250 |
| 434A -> 438A | -0.14734 |
| 422B -> 437B | 0.26700 |
| 423B -> 438B | 0.10702 |
| 429B -> 438B | 0.29166 |
| 430B -> 438B | 0.48769 |
| 431B -> 437B | -0.13250 |
| 434B -> 438B | -0.14734 |

Excited State 51: 3.000-A 1.5501 eV 799.83 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 427A -> 438A | 0.10442 |
| 428A -> 438A | 0.12409 |
| 429A -> 438A | 0.11232 |
| 430A -> 438A | -0.64748 |
| 431A -> 438A | -0.11076 |
| 427B -> 438B | -0.10442 |
| 428B -> 438B | -0.12409 |

429B -> 438B -0.11232
430B -> 438B 0.64748
431B -> 438B 0.11076

Excited State 52: 1.000-A 1.5652 eV 792.15 nm f=0.0174 <S**2>=0.000
423A -> 438A 0.19042
429A -> 438A 0.42043
430A -> 438A -0.41491
431A -> 438A -0.21974
434A -> 438A -0.11576
423B -> 438B 0.19042
429B -> 438B 0.42043
430B -> 438B -0.41491
431B -> 438B -0.21974
434B -> 438B -0.11576

Excited State 53: 3.000-A 1.5760 eV 786.69 nm f=0.0000 <S**2>=2.000
428A -> 439A -0.23530
429A -> 439A -0.34940
431A -> 439A 0.53851
432A -> 439A 0.12355
428B -> 439B 0.23530
429B -> 439B 0.34940
431B -> 439B -0.53851
432B -> 439B -0.12355

Excited State 54: 1.000-A 1.5926 eV 778.52 nm f=0.0124 <S**2>=0.000
423A -> 437A 0.27433
423A -> 438A 0.57308
425A -> 438A -0.10408
429A -> 438A -0.17287
431A -> 438A 0.10430
423B -> 437B 0.27433
423B -> 438B 0.57308
425B -> 438B -0.10408
429B -> 438B -0.17287

431B -> 438B 0.10430

Excited State 55: 3.000-A 1.5939 eV 777.86 nm f=0.0000 <S**2>=2.000
428A -> 439A -0.39627
429A -> 439A 0.51627
431A -> 439A 0.19419
432A -> 439A -0.16183
428B -> 439B 0.39627
429B -> 439B -0.51627
431B -> 439B -0.19419
432B -> 439B 0.16183

Excited State 56: 1.000-A 1.5985 eV 775.64 nm f=0.0013 <S**2>=0.000
428A -> 439A -0.39801
429A -> 439A -0.33302
430A -> 439A -0.14296
431A -> 439A 0.42555
428B -> 439B -0.39801
429B -> 439B -0.33302
430B -> 439B -0.14296
431B -> 439B 0.42555

Excited State 57: 3.000-A 1.6037 eV 773.13 nm f=0.0000 <S**2>=2.000
426A -> 437A 0.15261
427A -> 437A 0.36846
427A -> 438A -0.22784
428A -> 437A -0.29492
428A -> 438A -0.37578
430A -> 438A -0.16859
426B -> 437B -0.15261
427B -> 437B -0.36846
427B -> 438B 0.22784
428B -> 437B 0.29492
428B -> 438B 0.37578
430B -> 438B 0.16859

Excited State 58: 1.000-A 1.6096 eV 770.29 nm f=0.0002 <S**2>=0.000

| | |
|---|---|
| 428A -> 439A | -0.37694 |
| 429A -> 439A | 0.56851 |
| 431A -> 439A | 0.10813 |
| 432A -> 439A | -0.12028 |
| 428B -> 439B | -0.37694 |
| 429B -> 439B | 0.56851 |
| 431B -> 439B | 0.10813 |
| 432B -> 439B | -0.12028 |

Excited State 59: 1.000-A 1.6309 eV 760.23 nm f=0.0187 <S**2>=0.000

| | |
|---|---|
| 425A -> 439A | 0.65028 |
| 426A -> 439A | -0.12471 |
| 430A -> 439A | -0.10907 |
| 433A -> 439A | 0.10232 |
| 425B -> 439B | 0.65028 |
| 426B -> 439B | -0.12471 |
| 430B -> 439B | -0.10907 |
| 433B -> 439B | 0.10232 |

Excited State 60: 1.000-A 1.6397 eV 756.16 nm f=0.0021 <S**2>=0.000

| | |
|---|---|
| 427A -> 437A | -0.18052 |
| 427A -> 438A | 0.19674 |
| 428A -> 437A | 0.14804 |
| 428A -> 438A | 0.61102 |
| 430A -> 438A | 0.11356 |
| 427B -> 437B | -0.18052 |
| 427B -> 438B | 0.19674 |
| 428B -> 437B | 0.14804 |
| 428B -> 438B | 0.61102 |
| 430B -> 438B | 0.11356 |

Excited State 61: 3.000-A 1.6497 eV 751.54 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 426A -> 437A | -0.16305 |
| 427A -> 437A | -0.41021 |
| 428A -> 438A | -0.52313 |

426B -> 437B 0.16305
427B -> 437B 0.41021
428B -> 438B 0.52313

Excited State 62: 1.000-A 1.6811 eV 737.51 nm f=0.0009 <S**2>=0.000
426A -> 437A 0.21294
427A -> 437A 0.59004
428A -> 437A -0.12490
428A -> 438A 0.26397
426B -> 437B 0.21294
427B -> 437B 0.59004
428B -> 437B -0.12490
428B -> 438B 0.26397

Excited State 63: 3.000-A 1.7791 eV 696.91 nm f=0.0000 <S**2>=2.000
421A -> 438A -0.13131
426A -> 438A -0.19364
427A -> 437A -0.18353
427A -> 438A -0.55857
428A -> 438A 0.17136
429A -> 438A 0.16265
421B -> 438B 0.13131
426B -> 438B 0.19364
427B -> 437B 0.18353
427B -> 438B 0.55857
428B -> 438B -0.17136
429B -> 438B -0.16265

Excited State 64: 1.000-A 1.8304 eV 677.38 nm f=0.0013 <S**2>=0.000
426A -> 438A 0.21100
427A -> 437A 0.16931
427A -> 438A 0.61327
428A -> 438A -0.17201
426B -> 438B 0.21100
427B -> 437B 0.16931
427B -> 438B 0.61327

428B -> 438B -0.17201

Excited State 65: 3.000-A 1.8437 eV 672.47 nm f=0.0000 <S**2>=2.000
398A -> 437A 0.11153
401A -> 437A -0.12519
418A -> 437A -0.11752
419A -> 437A -0.25442
424A -> 437A 0.51748
424A -> 438A -0.13029
427A -> 437A -0.14198
398B -> 437B -0.11153
401B -> 437B 0.12519
418B -> 437B 0.11752
419B -> 437B 0.25442
424B -> 437B -0.51748
424B -> 438B 0.13029
427B -> 437B 0.14198

Excited State 66: 3.000-A 1.8874 eV 656.90 nm f=0.0000 <S**2>=2.000
408A -> 439A -0.14370
417A -> 439A -0.13708
420A -> 439A 0.27873
421A -> 439A 0.10324
426A -> 439A 0.32649
427A -> 439A -0.40733
408B -> 439B 0.14370
417B -> 439B 0.13708
420B -> 439B -0.27873
421B -> 439B -0.10324
426B -> 439B -0.32649
427B -> 439B 0.40733

Excited State 67: 3.000-A 1.8904 eV 655.85 nm f=0.0000 <S**2>=2.000
399A -> 438A -0.10121
400A -> 438A 0.11833
402A -> 438A -0.10674

403A -> 438A 0.15834
406A -> 438A -0.18764
410A -> 438A -0.12251
414A -> 438A 0.17708
416A -> 438A -0.19028
419A -> 438A 0.13175
420A -> 438A 0.10807
421A -> 438A -0.20221
424A -> 437A 0.11368
424A -> 438A 0.17937
427A -> 438A 0.14760
399B -> 438B 0.10121
400B -> 438B -0.11833
402B -> 438B 0.10674
403B -> 438B -0.15834
406B -> 438B 0.18764
410B -> 438B 0.12251
414B -> 438B -0.17708
416B -> 438B 0.19028
419B -> 438B -0.13175
420B -> 438B -0.10807
421B -> 438B 0.20221
424B -> 437B -0.11368
424B -> 438B -0.17937
427B -> 438B -0.14760

Excited State 68: 3.000-A 1.9143 eV 647.69 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.11000
401A -> 437A 0.15637
409A -> 437A -0.13090
411A -> 437A 0.13429
413A -> 437A -0.16258
415A -> 437A 0.11738
416A -> 437A 0.13750
421A -> 437A -0.20322
424A -> 437A 0.18271

426A -> 437A 0.41155
427A -> 437A -0.12406
398B -> 437B 0.11000
401B -> 437B -0.15637
409B -> 437B 0.13090
411B -> 437B -0.13429
413B -> 437B 0.16258
415B -> 437B -0.11738
416B -> 437B -0.13750
421B -> 437B 0.20322
424B -> 437B -0.18271
426B -> 437B -0.41155
427B -> 437B 0.12406

Excited State 69: 3.000-A 1.9198 eV 645.83 nm f=0.0000 <S**2>=2.000
408A -> 439A 0.17004
409A -> 439A -0.11220
411A -> 439A -0.12231
414A -> 439A -0.21845
416A -> 439A -0.11621
417A -> 439A 0.21549
420A -> 439A -0.30410
426A -> 439A 0.29172
427A -> 439A -0.29043
408B -> 439B -0.17004
409B -> 439B 0.11220
411B -> 439B 0.12231
414B -> 439B 0.21845
416B -> 439B 0.11621
417B -> 439B -0.21549
420B -> 439B 0.30410
426B -> 439B -0.29172
427B -> 439B 0.29043

Excited State 70: 1.000-A 1.9339 eV 641.11 nm f=0.0002 <S**2>=0.000
421A -> 437A -0.11600

424A -> 437A -0.15150
426A -> 437A 0.62892
427A -> 437A -0.21924
421B -> 437B -0.11600
424B -> 437B -0.15150
426B -> 437B 0.62892
427B -> 437B -0.21924

Excited State 71: 3.000-A 1.9362 eV 640.36 nm f=0.0000 <S**2>=2.000
416A -> 437A -0.10579
419A -> 437A -0.12929
424A -> 437A -0.34014
424A -> 438A 0.10473
426A -> 437A 0.44562
427A -> 437A -0.17541
416B -> 437B 0.10579
419B -> 437B 0.12929
424B -> 437B 0.34014
424B -> 438B -0.10473
426B -> 437B -0.44562
427B -> 437B 0.17541

Excited State 72: 3.000-A 1.9511 eV 635.45 nm f=0.0000 <S**2>=2.000
424A -> 438A 0.10857
425A -> 437A -0.39433
425A -> 438A -0.53031
426A -> 438A 0.13187
424B -> 438B -0.10857
425B -> 437B 0.39433
425B -> 438B 0.53031
426B -> 438B -0.13187

Excited State 73: 1.000-A 1.9515 eV 635.33 nm f=0.0087 <S**2>=0.000
424A -> 437A 0.64031
425A -> 437A -0.13153
425A -> 438A -0.14017

426A -> 437A 0.14348
424B -> 437B 0.64031
425B -> 437B -0.13153
425B -> 438B -0.14017
426B -> 437B 0.14348

Excited State 74: 1.000-A 1.9613 eV 632.15 nm f=0.0020 <S**2>=0.000
424A -> 437A 0.18531
425A -> 437A 0.39900
425A -> 438A 0.51919
426A -> 438A -0.11042
424B -> 437B 0.18531
425B -> 437B 0.39900
425B -> 438B 0.51919
426B -> 438B -0.11042

Excited State 75: 1.000-A 1.9960 eV 621.16 nm f=0.0141 <S**2>=0.000
426A -> 439A -0.19005
427A -> 439A 0.66807
426B -> 439B -0.19005
427B -> 439B 0.66807

Excited State 76: 3.000-A 2.0080 eV 617.46 nm f=0.0000 <S**2>=2.000
410A -> 439A 0.11264
419A -> 439A -0.15075
424A -> 439A -0.12566
426A -> 439A -0.45262
427A -> 439A -0.43461
410B -> 439B -0.11264
419B -> 439B 0.15075
424B -> 439B 0.12566
426B -> 439B 0.45262
427B -> 439B 0.43461

Excited State 77: 3.000-A 2.0414 eV 607.36 nm f=0.0000 <S**2>=2.000
407A -> 439A -0.11944

408A -> 439A -0.26380
410A -> 439A -0.32793
414A -> 439A -0.23083
415A -> 439A 0.10577
416A -> 439A -0.15275
418A -> 439A -0.18290
420A -> 439A -0.12120
421A -> 439A 0.18404
424A -> 439A 0.16938
426A -> 439A -0.20408
407B -> 439B 0.11944
408B -> 439B 0.26380
410B -> 439B 0.32793
414B -> 439B 0.23083
415B -> 439B -0.10577
416B -> 439B 0.15275
418B -> 439B 0.18290
420B -> 439B 0.12120
421B -> 439B -0.18404
424B -> 439B -0.16938
426B -> 439B 0.20408

Excited State 78: 3.000-A 2.0426 eV 606.98 nm f=0.0000 <S**2>=2.000
419A -> 438A -0.10962
421A -> 438A -0.10443
424A -> 437A 0.13766
424A -> 438A 0.53822
425A -> 437A 0.11673
426A -> 438A 0.18318
419B -> 438B 0.10962
421B -> 438B 0.10443
424B -> 437B -0.13766
424B -> 438B -0.53822
425B -> 437B -0.11673
426B -> 438B -0.18318

Excited State 79: 1.000-A 2.0549 eV 603.36 nm f=0.0062 <S**2>=0.000

| | |
|---|---|
| 425A -> 439A | 0.12671 |
| 426A -> 439A | 0.65430 |
| 427A -> 439A | 0.19376 |
| 425B -> 439B | 0.12671 |
| 426B -> 439B | 0.65430 |
| 427B -> 439B | 0.19376 |

Excited State 80: 3.000-A 2.0707 eV 598.75 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 402A -> 437A | 0.19665 |
| 405A -> 437A | 0.15789 |
| 409A -> 437A | -0.21737 |
| 411A -> 437A | 0.25269 |
| 415A -> 437A | -0.11276 |
| 420A -> 437A | 0.11367 |
| 421A -> 437A | 0.41068 |
| 402B -> 437B | -0.19665 |
| 405B -> 437B | -0.15789 |
| 409B -> 437B | 0.21737 |
| 411B -> 437B | -0.25269 |
| 415B -> 437B | 0.11276 |
| 420B -> 437B | -0.11367 |
| 421B -> 437B | -0.41068 |

Excited State 81: 3.000-A 2.0849 eV 594.68 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 395A -> 438A | 0.10609 |
| 405A -> 437A | -0.10260 |
| 405A -> 438A | -0.18626 |
| 406A -> 438A | 0.12315 |
| 407A -> 438A | 0.22094 |
| 409A -> 438A | -0.24499 |
| 414A -> 438A | 0.16794 |
| 416A -> 438A | -0.17065 |
| 417A -> 438A | -0.17209 |
| 418A -> 438A | 0.14825 |
| 424A -> 438A | 0.21356 |

425A -> 437A -0.10206
426A -> 438A -0.10567
395B -> 438B -0.10609
405B -> 437B 0.10260
405B -> 438B 0.18626
406B -> 438B -0.12315
407B -> 438B -0.22094
409B -> 438B 0.24499
414B -> 438B -0.16794
416B -> 438B 0.17065
417B -> 438B 0.17209
418B -> 438B -0.14825
424B -> 438B -0.21356
425B -> 437B 0.10206
426B -> 438B 0.10567

Excited State 82: 3.000-A 2.0894 eV 593.39 nm f=0.0000 <S**2>=2.000
419A -> 437A -0.11486
419A -> 438A 0.12492
421A -> 438A 0.10087
424A -> 438A 0.17145
425A -> 438A -0.10698
426A -> 437A -0.11510
426A -> 438A -0.54880
427A -> 438A 0.20877
419B -> 437B 0.11486
419B -> 438B -0.12492
421B -> 438B -0.10087
424B -> 438B -0.17145
425B -> 438B 0.10698
426B -> 437B 0.11510
426B -> 438B 0.54880
427B -> 438B -0.20877

Excited State 83: 1.000-A 2.0900 eV 593.22 nm f=0.0116 <S**2>=0.000
421A -> 437A -0.26979

424A -> 438A 0.46729
426A -> 438A -0.37553
427A -> 438A 0.15735
421B -> 437B -0.26979
424B -> 438B 0.46729
426B -> 438B -0.37553
427B -> 438B 0.15735

Excited State 84: 1.000-A 2.1045 eV 589.15 nm f=0.0183 <S**2>=0.000
421A -> 437A -0.16888
421A -> 438A -0.12032
424A -> 438A 0.35780
425A -> 437A 0.12713
426A -> 438A 0.51422
427A -> 438A -0.15543
421B -> 437B -0.16888
421B -> 438B -0.12032
424B -> 438B 0.35780
425B -> 437B 0.12713
426B -> 438B 0.51422
427B -> 438B -0.15543

Excited State 85: 1.000-A 2.1118 eV 587.11 nm f=0.0018 <S**2>=0.000
416A -> 437A -0.11358
421A -> 437A 0.58139
424A -> 438A 0.34020
416B -> 437B -0.11358
421B -> 437B 0.58139
424B -> 438B 0.34020

Excited State 86: 3.000-A 2.1167 eV 585.74 nm f=0.0000 <S**2>=2.000
402A -> 437A -0.15199
415A -> 437A 0.12568
419A -> 437A 0.28602
421A -> 437A 0.43990
425A -> 437A -0.10908

426A -> 437A 0.14545
426A -> 438A -0.18046
402B -> 437B 0.15199
415B -> 437B -0.12568
419B -> 437B -0.28602
421B -> 437B -0.43990
425B -> 437B 0.10908
426B -> 437B -0.14545
426B -> 438B 0.18046

Excited State 87: 3.000-A 2.1208 eV 584.60 nm f=0.0000 <S**2>=2.000
408A -> 439A 0.11755
409A -> 439A -0.11050
415A -> 439A -0.11985
418A -> 439A 0.12257
419A -> 439A 0.19892
420A -> 439A 0.27817
424A -> 439A 0.47531
426A -> 439A -0.12849
427A -> 439A -0.10905
408B -> 439B -0.11755
409B -> 439B 0.11050
415B -> 439B 0.11985
418B -> 439B -0.12257
419B -> 439B -0.19892
420B -> 439B -0.27817
424B -> 439B -0.47531
426B -> 439B 0.12849
427B -> 439B 0.10905

Excited State 88: 3.000-A 2.1269 eV 582.94 nm f=0.0000 <S**2>=2.000
421A -> 437A 0.11367
425A -> 437A 0.53672
425A -> 438A -0.40492
421B -> 437B -0.11367
425B -> 437B -0.53672

425B -> 438B 0.40492

Excited State 89: 1.000-A 2.1272 eV 582.86 nm f=0.0013 <S**2>=0.000
425A -> 437A 0.54371
425A -> 438A -0.42570
425B -> 437B 0.54371
425B -> 438B -0.42570

Excited State 90: 3.000-A 2.1571 eV 574.77 nm f=0.0000 <S**2>=2.000
397A -> 437A -0.11105
398A -> 437A 0.23121
401A -> 437A -0.26926
402A -> 437A 0.16426
413A -> 437A -0.22344
415A -> 437A -0.18198
419A -> 437A 0.35959
397B -> 437B 0.11105
398B -> 437B -0.23121
401B -> 437B 0.26926
402B -> 437B -0.16426
413B -> 437B 0.22344
415B -> 437B 0.18198
419B -> 437B -0.35959

Excited State 91: 3.000-A 2.1615 eV 573.60 nm f=0.0000 <S**2>=2.000
406A -> 438A 0.10933
410A -> 438A 0.11190
414A -> 438A -0.10190
416A -> 438A -0.10164
419A -> 437A 0.16129
421A -> 438A -0.53628
424A -> 438A -0.12346
426A -> 438A -0.10131
427A -> 438A 0.11394
406B -> 438B -0.10933
410B -> 438B -0.11190

414B -> 438B 0.10190
416B -> 438B 0.10164
419B -> 437B -0.16129
421B -> 438B 0.53628
424B -> 438B 0.12346
426B -> 438B 0.10131
427B -> 438B -0.11394

Excited State 92: 1.000-A 2.1726 eV 570.67 nm f=0.0224 <S**2>=0.000
418A -> 437A 0.19279
419A -> 437A 0.60087
420A -> 437A -0.15227
421A -> 437A 0.10742
418B -> 437B 0.19279
419B -> 437B 0.60087
420B -> 437B -0.15227
421B -> 437B 0.10742

Excited State 93: 1.000-A 2.2037 eV 562.63 nm f=0.0057 <S**2>=0.000
419A -> 439A 0.16592
421A -> 438A 0.37354
421A -> 439A 0.17329
424A -> 439A 0.50104
419B -> 439B 0.16592
421B -> 438B 0.37354
421B -> 439B 0.17329
424B -> 439B 0.50104

Excited State 94: 1.000-A 2.2067 eV 561.85 nm f=0.0212 <S**2>=0.000
416A -> 437A 0.10643
419A -> 437A -0.11996
419A -> 439A -0.10372
421A -> 438A 0.49964
421A -> 439A -0.14987
424A -> 439A -0.35726
416B -> 437B 0.10643

419B -> 437B -0.11996
419B -> 439B -0.10372
421B -> 438B 0.49964
421B -> 439B -0.14987
424B -> 439B -0.35726

Excited State 95: 3.000-A 2.2189 eV 558.77 nm f=0.0000 <S**2>=2.000
433A -> 440A -0.18940
435A -> 440A -0.13954
436A -> 440A 0.66216
433B -> 440B 0.18940
435B -> 440B 0.13954
436B -> 440B -0.66216

Excited State 96: 1.000-A 2.2256 eV 557.07 nm f=0.0002 <S**2>=0.000
433A -> 440A -0.17651
435A -> 440A -0.12311
436A -> 440A 0.67097
433B -> 440B -0.17651
435B -> 440B -0.12311
436B -> 440B 0.67097

Excited State 97: 3.000-A 2.2477 eV 551.61 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.11872
402A -> 437A 0.25590
414A -> 437A 0.16445
415A -> 437A 0.30716
416A -> 437A 0.11247
419A -> 437A -0.19613
420A -> 437A -0.29368
393B -> 437B 0.11872
402B -> 437B -0.25590
414B -> 437B -0.16445
415B -> 437B -0.30716
416B -> 437B -0.11247
419B -> 437B 0.19613

420B -> 437B 0.29368

Excited State 98: 1.000-A 2.2549 eV 549.84 nm f=0.0011 <S**2>=0.000
415A -> 437A 0.33979
415A -> 438A -0.10477
416A -> 437A 0.13462
416A -> 438A -0.10405
417A -> 437A -0.14213
417A -> 438A -0.15650
418A -> 437A 0.16207
418A -> 438A 0.15372
419A -> 437A -0.19958
419A -> 438A -0.13582
420A -> 437A -0.32767
421A -> 438A -0.18334
415B -> 437B 0.33979
415B -> 438B -0.10477
416B -> 437B 0.13462
416B -> 438B -0.10405
417B -> 437B -0.14213
417B -> 438B -0.15650
418B -> 437B 0.16207
418B -> 438B 0.15372
419B -> 437B -0.19958
419B -> 438B -0.13582
420B -> 437B -0.32767
421B -> 438B -0.18334

Excited State 99: 3.000-A 2.2561 eV 549.54 nm f=0.0000 <S**2>=2.000
410A -> 439A 0.11742
414A -> 439A 0.28140
415A -> 439A -0.11813
416A -> 439A 0.11534
417A -> 439A -0.21290
418A -> 439A -0.17534
419A -> 439A 0.21978

420A -> 439A -0.40063
424A -> 439A 0.15946
410B -> 439B -0.11742
414B -> 439B -0.28140
415B -> 439B 0.11813
416B -> 439B -0.11534
417B -> 439B 0.21290
418B -> 439B 0.17534
419B -> 439B -0.21978
420B -> 439B 0.40063
424B -> 439B -0.15946

Excited State 100: 3.000-A 2.2631 eV 547.86 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.10905
395A -> 438A -0.29884
397A -> 438A 0.11790
402A -> 437A -0.15506
406A -> 438A -0.13117
407A -> 438A -0.13832
415A -> 437A -0.18201
416A -> 437A -0.12490
417A -> 437A -0.10130
417A -> 438A -0.21369
418A -> 437A 0.10402
418A -> 438A 0.19080
419A -> 438A -0.24015
420A -> 438A -0.10063
395B -> 437B 0.10905
395B -> 438B 0.29884
397B -> 438B -0.11790
402B -> 437B 0.15506
406B -> 438B 0.13117
407B -> 438B 0.13832
415B -> 437B 0.18201
416B -> 437B 0.12490
417B -> 437B 0.10130

417B -> 438B 0.21369
418B -> 437B -0.10402
418B -> 438B -0.19080
419B -> 438B 0.24015
420B -> 438B 0.10063

Excited State 101: 3.000-A 2.2674 eV 546.81 nm f=0.0000 <S**2>=2.000
423A -> 437A 0.63629
423A -> 438A -0.28464
423B -> 437B -0.63629
423B -> 438B 0.28464

Excited State 102: 1.000-A 2.2686 eV 546.53 nm f=0.0001 <S**2>=0.000
423A -> 437A 0.63331
423A -> 438A -0.30281
423B -> 437B 0.63331
423B -> 438B -0.30281

Excited State 103: 1.000-A 2.2709 eV 545.97 nm f=0.0047 <S**2>=0.000
413A -> 437A 0.15439
415A -> 437A 0.39681
416A -> 437A 0.19825
417A -> 437A 0.12338
417A -> 438A 0.25745
418A -> 437A -0.12598
418A -> 438A -0.25072
419A -> 438A 0.22457
420A -> 438A 0.15292
413B -> 437B 0.15439
415B -> 437B 0.39681
416B -> 437B 0.19825
417B -> 437B 0.12338
417B -> 438B 0.25745
418B -> 437B -0.12598
418B -> 438B -0.25072
419B -> 438B 0.22457

420B -> 438B 0.15292

Excited State 104: 3.000-A 2.2805 eV 543.67 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.10874
395A -> 438A -0.11621
401A -> 437A -0.14441
410A -> 437A 0.13146
412A -> 437A -0.15121
413A -> 437A 0.22356
414A -> 437A -0.16732
415A -> 437A 0.30205
419A -> 437A 0.11915
420A -> 437A 0.35089
393B -> 437B 0.10874
395B -> 438B 0.11621
401B -> 437B 0.14441
410B -> 437B -0.13146
412B -> 437B 0.15121
413B -> 437B -0.22356
414B -> 437B 0.16732
415B -> 437B -0.30205
419B -> 437B -0.11915
420B -> 437B -0.35089

Excited State 105: 3.000-A 2.2856 eV 542.45 nm f=0.0000 <S**2>=2.000
407A -> 439A -0.11825
409A -> 439A -0.13554
410A -> 439A -0.10829
418A -> 439A -0.14626
420A -> 439A 0.11108
421A -> 439A -0.55615
424A -> 439A -0.14243
407B -> 439B 0.11825
409B -> 439B 0.13554
410B -> 439B 0.10829
418B -> 439B 0.14626

420B -> 439B -0.11108
421B -> 439B 0.55615
424B -> 439B 0.14243

Excited State 106: 3.000-A 2.2873 eV 542.04 nm f=0.0000 <S**2>=2.000
398A -> 437A -0.20000
401A -> 437A 0.15285
402A -> 437A 0.31552
406A -> 437A -0.10927
409A -> 437A 0.14587
410A -> 437A -0.10915
413A -> 437A 0.24192
415A -> 437A -0.13600
416A -> 437A -0.18658
419A -> 437A 0.13933
420A -> 437A 0.11024
398B -> 437B 0.20000
401B -> 437B -0.15285
402B -> 437B -0.31552
406B -> 437B 0.10927
409B -> 437B -0.14587
410B -> 437B 0.10915
413B -> 437B -0.24192
415B -> 437B 0.13600
416B -> 437B 0.18658
419B -> 437B -0.13933
420B -> 437B -0.11024

Excited State 107: 1.000-A 2.2892 eV 541.61 nm f=0.0185 <S**2>=0.000
408A -> 439A -0.11999
417A -> 439A -0.10665
418A -> 439A -0.18954
420A -> 439A -0.38560
421A -> 439A 0.46654
424A -> 439A -0.15464
408B -> 439B -0.11999

417B -> 439B -0.10665
418B -> 439B -0.18954
420B -> 439B -0.38560
421B -> 439B 0.46654
424B -> 439B -0.15464

Excited State 108: 1.000-A 2.2990 eV 539.29 nm f=0.0006 <S**2>=0.000
410A -> 437A 0.10867
413A -> 437A 0.21077
414A -> 437A -0.15256
415A -> 437A 0.18668
417A -> 437A -0.10983
417A -> 438A -0.18168
418A -> 437A 0.11460
418A -> 438A 0.15327
419A -> 438A -0.12078
420A -> 437A 0.48706
410B -> 437B 0.10867
413B -> 437B 0.21077
414B -> 437B -0.15256
415B -> 437B 0.18668
417B -> 437B -0.10983
417B -> 438B -0.18168
418B -> 437B 0.11460
418B -> 438B 0.15327
419B -> 438B -0.12078
420B -> 437B 0.48706

Excited State 109: 3.000-A 2.3023 eV 538.51 nm f=0.0000 <S**2>=2.000
403A -> 438A -0.10816
407A -> 437A -0.10849
407A -> 438A -0.16917
408A -> 438A 0.16669
413A -> 437A -0.16588
415A -> 438A 0.10701
416A -> 437A -0.13199

416A -> 438A -0.29252
417A -> 438A 0.15348
419A -> 438A 0.26251
420A -> 437A -0.10704
421A -> 438A 0.11364
403B -> 438B 0.10816
407B -> 437B 0.10849
407B -> 438B 0.16917
408B -> 438B -0.16669
413B -> 437B 0.16588
415B -> 438B -0.10701
416B -> 437B 0.13199
416B -> 438B 0.29252
417B -> 438B -0.15348
419B -> 438B -0.26251
420B -> 437B 0.10704
421B -> 438B -0.11364

Excited State 110: 3.000-A 2.3095 eV 536.84 nm f=0.0000 <S**2>=2.000
434A -> 440A -0.18498
435A -> 440A -0.65467
436A -> 440A -0.16231
434B -> 440B 0.18498
435B -> 440B 0.65467
436B -> 440B 0.16231

Excited State 111: 1.000-A 2.3113 eV 536.44 nm f=0.0002 <S**2>=0.000
434A -> 440A 0.18385
435A -> 440A 0.66305
436A -> 440A 0.14054
434B -> 440B 0.18385
435B -> 440B 0.66305
436B -> 440B 0.14054

Excited State 112: 1.000-A 2.3169 eV 535.12 nm f=0.0260 <S**2>=0.000
418A -> 439A 0.13513

419A -> 439A -0.10056
420A -> 439A 0.47286
421A -> 439A 0.42147
424A -> 439A -0.18913
418B -> 439B 0.13513
419B -> 439B -0.10056
420B -> 439B 0.47286
421B -> 439B 0.42147
424B -> 439B -0.18913

Excited State 113: 3.000-A 2.3244 eV 533.40 nm f=0.0000 <S**2>=2.000
395A -> 438A 0.18611
397A -> 438A -0.11369
407A -> 438A -0.15899
408A -> 438A 0.10108
413A -> 438A -0.10318
414A -> 438A 0.15809
415A -> 438A 0.11887
416A -> 437A -0.11425
418A -> 438A -0.15156
419A -> 438A -0.42108
420A -> 437A 0.12195
421A -> 438A -0.10830
426A -> 438A -0.12594
395B -> 438B -0.18611
397B -> 438B 0.11369
407B -> 438B 0.15899
408B -> 438B -0.10108
413B -> 438B 0.10318
414B -> 438B -0.15809
415B -> 438B -0.11887
416B -> 437B 0.11425
418B -> 438B 0.15156
419B -> 438B 0.42108
420B -> 437B -0.12195
421B -> 438B 0.10830

426B -> 438B 0.12594

Excited State 114: 3.000-A 2.3396 eV 529.95 nm f=0.0000 <S**2>=2.000
395A -> 438A 0.15221
408A -> 438A -0.11412
409A -> 437A 0.16676
412A -> 437A 0.12335
413A -> 437A -0.22980
414A -> 438A -0.14292
416A -> 437A -0.11838
417A -> 437A -0.16028
417A -> 438A -0.17432
418A -> 437A 0.17241
418A -> 438A 0.14077
419A -> 437A -0.11480
420A -> 437A 0.27444
420A -> 438A 0.21461
395B -> 438B -0.15221
408B -> 438B 0.11412
409B -> 437B -0.16676
412B -> 437B -0.12335
413B -> 437B 0.22980
414B -> 438B 0.14292
416B -> 437B 0.11838
417B -> 437B 0.16028
417B -> 438B 0.17432
418B -> 437B -0.17241
418B -> 438B -0.14077
419B -> 437B 0.11480
420B -> 437B -0.27444
420B -> 438B -0.21461

Excited State 115: 3.000-A 2.3550 eV 526.46 nm f=0.0000 <S**2>=2.000
396A -> 439A -0.10689
399A -> 439A 0.13539
407A -> 439A 0.11925

409A -> 439A 0.15816
413A -> 439A -0.11255
414A -> 439A -0.10929
415A -> 439A 0.13382
416A -> 439A -0.16033
419A -> 439A -0.24025
421A -> 439A -0.29486
424A -> 439A 0.36669
396B -> 439B 0.10689
399B -> 439B -0.13539
407B -> 439B -0.11925
409B -> 439B -0.15816
413B -> 439B 0.11255
414B -> 439B 0.10929
415B -> 439B -0.13382
416B -> 439B 0.16033
419B -> 439B 0.24025
421B -> 439B 0.29486
424B -> 439B -0.36669

Excited State 116: 3.000-A 2.3575 eV 525.91 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.11320
395A -> 438A -0.27916
397A -> 438A 0.10959
405A -> 438A -0.10063
407A -> 438A 0.15991
409A -> 438A -0.16900
412A -> 437A 0.11948
413A -> 437A -0.20344
414A -> 437A 0.11920
415A -> 437A 0.10394
416A -> 438A 0.17321
417A -> 438A 0.12236
418A -> 438A -0.16657
420A -> 437A 0.20989
395B -> 437B 0.11320

395B -> 438B 0.27916
397B -> 438B -0.10959
405B -> 438B 0.10063
407B -> 438B -0.15991
409B -> 438B 0.16900
412B -> 437B -0.11948
413B -> 437B 0.20344
414B -> 437B -0.11920
415B -> 437B -0.10394
416B -> 438B -0.17321
417B -> 438B -0.12236
418B -> 438B 0.16657
420B -> 437B -0.20989

Excited State 117: 1.000-A 2.3582 eV 525.76 nm f=0.0048 <S**2>=0.000
413A -> 437A 0.14641
416A -> 437A -0.20836
416A -> 438A -0.23189
418A -> 438A 0.18441
419A -> 438A 0.49133
420A -> 437A -0.11216
421A -> 438A 0.14621
413B -> 437B 0.14641
416B -> 437B -0.20836
416B -> 438B -0.23189
418B -> 438B 0.18441
419B -> 438B 0.49133
420B -> 437B -0.11216
421B -> 438B 0.14621

Excited State 118: 1.000-A 2.3604 eV 525.27 nm f=0.0041 <S**2>=0.000
408A -> 439A 0.18675
410A -> 439A 0.21236
414A -> 439A 0.12754
417A -> 439A 0.25918
418A -> 439A 0.36822

419A -> 439A -0.11649
420A -> 438A -0.11477
420A -> 439A -0.26823
421A -> 439A 0.14970
423A -> 439A 0.13495
408B -> 439B 0.18675
410B -> 439B 0.21236
414B -> 439B 0.12754
417B -> 439B 0.25918
418B -> 439B 0.36822
419B -> 439B -0.11649
420B -> 438B -0.11477
420B -> 439B -0.26823
421B -> 439B 0.14970
423B -> 439B 0.13495

Excited State 119: 1.000-A 2.3674 eV 523.71 nm f=0.0216 <S**2>=0.000
413A -> 437A -0.36670
414A -> 437A 0.11418
417A -> 437A -0.16340
418A -> 437A 0.15234
419A -> 437A -0.11747
420A -> 437A 0.13139
420A -> 438A 0.41725
413B -> 437B -0.36670
414B -> 437B 0.11418
417B -> 437B -0.16340
418B -> 437B 0.15234
419B -> 437B -0.11747
420B -> 437B 0.13139
420B -> 438B 0.41725

Excited State 120: 3.000-A 2.3725 eV 522.60 nm f=0.0000 <S**2>=2.000
423A -> 439A -0.68547
423B -> 439B 0.68547

Excited State 121: 1.000-A 2.3738 eV 522.29 nm f=0.0003 <S**2>=0.000

| | |
|---|---|
| 423A -> 439A | 0.68480 |
| 423B -> 439B | 0.68480 |

Excited State 122: 3.000-A 2.3814 eV 520.63 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 393A -> 437A | -0.17364 |
| 409A -> 437A | 0.11129 |
| 412A -> 437A | 0.16867 |
| 415A -> 437A | 0.14644 |
| 416A -> 437A | -0.31152 |
| 416A -> 438A | 0.10387 |
| 417A -> 437A | 0.12411 |
| 419A -> 438A | 0.12377 |
| 420A -> 438A | -0.41196 |
| 393B -> 437B | 0.17364 |
| 409B -> 437B | -0.11129 |
| 412B -> 437B | -0.16867 |
| 415B -> 437B | -0.14644 |
| 416B -> 437B | 0.31152 |
| 416B -> 438B | -0.10387 |
| 417B -> 437B | -0.12411 |
| 419B -> 438B | -0.12377 |
| 420B -> 438B | 0.41196 |

Excited State 123: 1.000-A 2.3924 eV 518.25 nm f=0.0051 <S**2>=0.000

| | |
|---|---|
| 410A -> 437A | -0.13477 |
| 412A -> 437A | -0.12114 |
| 413A -> 437A | 0.31872 |
| 415A -> 437A | -0.29475 |
| 416A -> 437A | 0.33427 |
| 417A -> 437A | -0.16830 |
| 417A -> 438A | -0.10732 |
| 420A -> 438A | 0.27747 |
| 410B -> 437B | -0.13477 |
| 412B -> 437B | -0.12114 |
| 413B -> 437B | 0.31872 |

415B -> 437B -0.29475
416B -> 437B 0.33427
417B -> 437B -0.16830
417B -> 438B -0.10732
420B -> 438B 0.27747

Excited State 124: 3.000-A 2.4016 eV 516.25 nm f=0.0000 <S**2>=2.000
396A -> 439A -0.21997
397A -> 439A 0.12011
408A -> 439A 0.26495
410A -> 439A 0.11657
411A -> 439A -0.15578
414A -> 439A -0.24848
417A -> 439A -0.28083
418A -> 439A -0.29281
419A -> 439A 0.13273
420A -> 439A 0.10156
421A -> 439A 0.10527
423A -> 439A -0.11040
396B -> 439B 0.21997
397B -> 439B -0.12011
408B -> 439B -0.26495
410B -> 439B -0.11657
411B -> 439B 0.15578
414B -> 439B 0.24848
417B -> 439B 0.28083
418B -> 439B 0.29281
419B -> 439B -0.13273
420B -> 439B -0.10156
421B -> 439B -0.10527
423B -> 439B 0.11040

Excited State 125: 1.000-A 2.4031 eV 515.94 nm f=0.0091 <S**2>=0.000
413A -> 437A -0.17339
414A -> 437A -0.19707
415A -> 438A -0.11606

416A -> 437A 0.30089
416A -> 438A 0.13481
418A -> 437A 0.12975
419A -> 438A 0.29583
420A -> 437A 0.10732
420A -> 438A -0.27391
422A -> 438A 0.15170
413B -> 437B -0.17339
414B -> 437B -0.19707
415B -> 438B -0.11606
416B -> 437B 0.30089
416B -> 438B 0.13481
418B -> 437B 0.12975
419B -> 438B 0.29583
420B -> 437B 0.10732
420B -> 438B -0.27391
422B -> 438B 0.15170

Excited State 126: 3.000-A 2.4137 eV 513.68 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.14395
412A -> 437A 0.11733
420A -> 438A 0.16189
422A -> 437A -0.15530
422A -> 438A -0.61200
393B -> 437B 0.14395
412B -> 437B -0.11733
420B -> 438B -0.16189
422B -> 437B 0.15530
422B -> 438B 0.61200

Excited State 127: 3.000-A 2.4141 eV 513.58 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.27979
412A -> 437A -0.22275
413A -> 437A -0.16437
414A -> 437A 0.10309
416A -> 437A 0.11187

419A -> 438A 0.11081
420A -> 437A 0.16980
420A -> 438A -0.33345
422A -> 438A -0.30054
393B -> 437B -0.27979
412B -> 437B 0.22275
413B -> 437B 0.16437
414B -> 437B -0.10309
416B -> 437B -0.11187
419B -> 438B -0.11081
420B -> 437B -0.16980
420B -> 438B 0.33345
422B -> 438B 0.30054

Excited State 128: 1.000-A 2.4142 eV 513.55 nm f=0.0008 <S**2>=0.000
416A -> 437A -0.10065
422A -> 437A 0.15923
422A -> 438A 0.66517
416B -> 437B -0.10065
422B -> 437B 0.15923
422B -> 438B 0.66517

Excited State 129: 3.000-A 2.4387 eV 508.40 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.21176
410A -> 437A -0.12405
412A -> 437A 0.26841
413A -> 437A 0.10604
415A -> 437A -0.15226
416A -> 437A 0.26722
417A -> 437A -0.22881
417A -> 438A 0.12540
418A -> 437A 0.16816
419A -> 438A 0.10628
420A -> 437A 0.15218
420A -> 438A -0.20241
393B -> 437B 0.21176

410B -> 437B 0.12405
412B -> 437B -0.26841
413B -> 437B -0.10604
415B -> 437B 0.15226
416B -> 437B -0.26722
417B -> 437B 0.22881
417B -> 438B -0.12540
418B -> 437B -0.16816
419B -> 438B -0.10628
420B -> 437B -0.15218
420B -> 438B 0.20241

Excited State 130: 1.000-A 2.4446 eV 507.18 nm f=0.0045 <S**2>=0.000
410A -> 437A -0.15536
411A -> 437A -0.10214
414A -> 437A 0.48646
416A -> 437A 0.10033
417A -> 437A -0.11676
418A -> 437A -0.15540
420A -> 437A 0.20119
420A -> 438A -0.25559
410B -> 437B -0.15536
411B -> 437B -0.10214
414B -> 437B 0.48646
416B -> 437B 0.10033
417B -> 437B -0.11676
418B -> 437B -0.15540
420B -> 437B 0.20119
420B -> 438B -0.25559

Excited State 131: 1.000-A 2.4517 eV 505.70 nm f=0.0094 <S**2>=0.000
413A -> 439A 0.12131
415A -> 439A -0.13236
419A -> 439A 0.61681
424A -> 439A -0.18952
413B -> 439B 0.12131

415B -> 439B -0.13236
419B -> 439B 0.61681
424B -> 439B -0.18952

Excited State 132: 1.000-A 2.4521 eV 505.63 nm f=0.0208 <S**2>=0.000
401A -> 437A 0.10464
409A -> 437A 0.15607
411A -> 437A -0.21872
412A -> 437A 0.36505
413A -> 437A 0.10321
414A -> 437A 0.13930
415A -> 438A -0.13777
416A -> 438A 0.35593
401B -> 437B 0.10464
409B -> 437B 0.15607
411B -> 437B -0.21872
412B -> 437B 0.36505
413B -> 437B 0.10321
414B -> 437B 0.13930
415B -> 438B -0.13777
416B -> 438B 0.35593

Excited State 133: 3.000-A 2.4580 eV 504.40 nm f=0.0000 <S**2>=2.000
412A -> 437A -0.20033
414A -> 437A -0.16322
416A -> 437A -0.16904
417A -> 438A 0.25263
418A -> 437A 0.49539
418A -> 438A -0.14761
419A -> 437A -0.16449
412B -> 437B 0.20033
414B -> 437B 0.16322
416B -> 437B 0.16904
417B -> 438B -0.25263
418B -> 437B -0.49539
418B -> 438B 0.14761

419B -> 437B 0.16449

Excited State 134: 1.000-A 2.4610 eV 503.79 nm f=0.0006 <S**2>=0.000
413A -> 437A 0.14484
415A -> 437A -0.11918
415A -> 438A 0.11122
417A -> 437A -0.13538
417A -> 438A 0.32876
418A -> 437A 0.46227
418A -> 438A -0.17098
419A -> 437A -0.12887
413B -> 437B 0.14484
415B -> 437B -0.11918
415B -> 438B 0.11122
417B -> 437B -0.13538
417B -> 438B 0.32876
418B -> 437B 0.46227
418B -> 438B -0.17098
419B -> 437B -0.12887

Excited State 135: 1.000-A 2.4707 eV 501.81 nm f=0.0010 <S**2>=0.000
411A -> 437A -0.14006
416A -> 437A 0.20028
417A -> 437A 0.52614
418A -> 437A 0.18800
418A -> 438A 0.22901
411B -> 437B -0.14006
416B -> 437B 0.20028
417B -> 437B 0.52614
418B -> 437B 0.18800
418B -> 438B 0.22901

Excited State 136: 3.000-A 2.4724 eV 501.48 nm f=0.0000 <S**2>=2.000
416A -> 437A 0.22428
416A -> 438A -0.10334
417A -> 437A 0.54652

418A -> 437A 0.20209
418A -> 438A 0.21888
416B -> 437B -0.22428
416B -> 438B 0.10334
417B -> 437B -0.54652
418B -> 437B -0.20209
418B -> 438B -0.21888

Excited State 137: 3.000-A 2.4755 eV 500.85 nm f=0.0000 <S**2>=2.000
396A -> 439A 0.23912
397A -> 439A -0.13637
399A -> 439A -0.11744
400A -> 439A 0.11094
409A -> 439A -0.11942
416A -> 439A 0.13348
417A -> 439A -0.25991
418A -> 439A -0.18444
419A -> 439A -0.42404
396B -> 439B -0.23912
397B -> 439B 0.13637
399B -> 439B 0.11744
400B -> 439B -0.11094
409B -> 439B 0.11942
416B -> 439B -0.13348
417B -> 439B 0.25991
418B -> 439B 0.18444
419B -> 439B 0.42404

Excited State 138: 1.000-A 2.4791 eV 500.11 nm f=0.0064 <S**2>=0.000
409A -> 437A -0.11132
412A -> 437A 0.49602
412A -> 438A -0.10548
416A -> 437A 0.17051
416A -> 438A -0.28169
418A -> 437A -0.17086
409B -> 437B -0.11132

412B -> 437B 0.49602
412B -> 438B -0.10548
416B -> 437B 0.17051
416B -> 438B -0.28169
418B -> 437B -0.17086

Excited State 139: 3.000-A 2.4879 eV 498.35 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.12726
411A -> 440A 0.12155
412A -> 440A 0.56953
413A -> 440A 0.26016
415A -> 440A 0.15023
393B -> 437B -0.12726
411B -> 440B -0.12155
412B -> 440B -0.56953
413B -> 440B -0.26016
415B -> 440B -0.15023

Excited State 140: 1.000-A 2.4959 eV 496.76 nm f=0.0150 <S**2>=0.000
408A -> 439A -0.27268
410A -> 439A -0.24636
411A -> 439A 0.14429
415A -> 439A 0.12977
416A -> 439A -0.16199
417A -> 439A 0.48140
418A -> 439A 0.11996
408B -> 439B -0.27268
410B -> 439B -0.24636
411B -> 439B 0.14429
415B -> 439B 0.12977
416B -> 439B -0.16199
417B -> 439B 0.48140
418B -> 439B 0.11996

Excited State 141: 3.000-A 2.5034 eV 495.27 nm f=0.0000 <S**2>=2.000
409A -> 437A -0.17440

414A -> 437A 0.40587
414A -> 438A 0.12483
416A -> 438A 0.33528
418A -> 437A 0.17530
418A -> 438A 0.11447
409B -> 437B 0.17440
414B -> 437B -0.40587
414B -> 438B -0.12483
416B -> 438B -0.33528
418B -> 437B -0.17530
418B -> 438B -0.11447

Excited State 142: 1.000-A 2.5116 eV 493.64 nm f=0.0129 <S**2>=0.000
405A -> 438A 0.16827
406A -> 438A -0.13498
407A -> 438A -0.22325
409A -> 437A 0.28367
409A -> 438A 0.27769
411A -> 437A -0.17410
413A -> 438A -0.16478
415A -> 438A 0.16112
416A -> 438A -0.18937
405B -> 438B 0.16827
406B -> 438B -0.13498
407B -> 438B -0.22325
409B -> 437B 0.28367
409B -> 438B 0.27769
411B -> 437B -0.17410
413B -> 438B -0.16478
415B -> 438B 0.16112
416B -> 438B -0.18937

Excited State 143: 3.000-A 2.5148 eV 493.02 nm f=0.0000 <S**2>=2.000
408A -> 438A 0.12278
409A -> 437A 0.22161
409A -> 438A -0.11282

410A -> 438A -0.13759
411A -> 437A -0.12203
414A -> 437A -0.25815
414A -> 438A 0.30808
416A -> 437A 0.13648
416A -> 438A 0.18306
417A -> 438A -0.21231
419A -> 438A 0.16680
408B -> 438B -0.12278
409B -> 437B -0.22161
409B -> 438B 0.11282
410B -> 438B 0.13759
411B -> 437B 0.12203
414B -> 437B 0.25815
414B -> 438B -0.30808
416B -> 437B -0.13648
416B -> 438B -0.18306
417B -> 438B 0.21231
419B -> 438B -0.16680

Excited State 144: 3.000-A 2.5231 eV 491.39 nm f=0.0000 <S**2>=2.000
396A -> 439A 0.21212
410A -> 439A 0.15317
414A -> 439A 0.12713
415A -> 439A 0.14796
416A -> 439A -0.12883
417A -> 439A 0.28806
418A -> 439A -0.39888
419A -> 439A 0.16956
422A -> 439A -0.14712
396B -> 439B -0.21212
410B -> 439B -0.15317
414B -> 439B -0.12713
415B -> 439B -0.14796
416B -> 439B 0.12883
417B -> 439B -0.28806

418B -> 439B 0.39888
419B -> 439B -0.16956
422B -> 439B 0.14712

Excited State 145: 1.000-A 2.5262 eV 490.80 nm f=0.0000 <S**2>=0.000
422A -> 439A 0.69602
422B -> 439B 0.69602

Excited State 146: 3.000-A 2.5264 eV 490.76 nm f=0.0000 <S**2>=2.000
418A -> 439A 0.10983
422A -> 439A -0.68489
418B -> 439B -0.10983
422B -> 439B 0.68489

Excited State 147: 1.000-A 2.5270 eV 490.64 nm f=0.0007 <S**2>=0.000
407A -> 437A -0.11853
408A -> 437A 0.13544
409A -> 438A 0.15065
411A -> 437A 0.41553
412A -> 437A 0.10793
413A -> 437A 0.13417
413A -> 438A -0.12506
414A -> 437A 0.16040
414A -> 438A 0.16671
416A -> 438A 0.15624
417A -> 437A 0.13464
417A -> 438A -0.12518
418A -> 437A 0.14012
407B -> 437B -0.11853
408B -> 437B 0.13544
409B -> 438B 0.15065
411B -> 437B 0.41553
412B -> 437B 0.10793
413B -> 437B 0.13417
413B -> 438B -0.12506
414B -> 437B 0.16040

414B -> 438B 0.16671
416B -> 438B 0.15624
417B -> 437B 0.13464
417B -> 438B -0.12518
418B -> 437B 0.14012

Excited State 148: 3.000-A 2.5302 eV 490.01 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.29207
408A -> 437A 0.15736
410A -> 437A -0.20713
411A -> 437A 0.16441
412A -> 437A 0.35026
412A -> 440A -0.12901
413A -> 437A 0.18534
414A -> 437A -0.15386
415A -> 437A 0.14987
416A -> 438A 0.11103
393B -> 437B -0.29207
408B -> 437B -0.15736
410B -> 437B 0.20713
411B -> 437B -0.16441
412B -> 437B -0.35026
412B -> 440B 0.12901
413B -> 437B -0.18534
414B -> 437B 0.15386
415B -> 437B -0.14987
416B -> 438B -0.11103

Excited State 149: 1.000-A 2.5362 eV 488.85 nm f=0.0009 <S**2>=0.000
408A -> 439A -0.16213
410A -> 439A -0.19567
414A -> 438A -0.13472
417A -> 439A -0.36037
418A -> 439A 0.46920
408B -> 439B -0.16213
410B -> 439B -0.19567

414B -> 438B -0.13472
417B -> 439B -0.36037
418B -> 439B 0.46920

Excited State 150: 1.000-A 2.5388 eV 488.36 nm f=0.0085 <S**2>=0.000
408A -> 437A -0.14159
410A -> 437A 0.20301
414A -> 438A 0.40675
415A -> 438A 0.14105
416A -> 437A 0.11107
417A -> 438A -0.21015
417A -> 439A -0.11287
418A -> 438A -0.11355
418A -> 439A 0.17002
419A -> 438A 0.10604
408B -> 437B -0.14159
410B -> 437B 0.20301
414B -> 438B 0.40675
415B -> 438B 0.14105
416B -> 437B 0.11107
417B -> 438B -0.21015
417B -> 439B -0.11287
418B -> 438B -0.11355
418B -> 439B 0.17002
419B -> 438B 0.10604

Excited State 151: 3.000-A 2.5401 eV 488.11 nm f=0.0000 <S**2>=2.000
396A -> 439A 0.24741
397A -> 439A -0.11635
407A -> 439A 0.13731
416A -> 439A -0.35160
417A -> 439A -0.34924
418A -> 439A 0.24925
419A -> 439A 0.19352
396B -> 439B -0.24741
397B -> 439B 0.11635

407B -> 439B -0.13731
416B -> 439B 0.35160
417B -> 439B 0.34924
418B -> 439B -0.24925
419B -> 439B -0.19352

Excited State 152: 3.000-A 2.5522 eV 485.79 nm f=0.0000 <S**2>=2.000
393A -> 437A -0.11181
398A -> 437A -0.10088
405A -> 437A -0.21414
407A -> 437A -0.10152
408A -> 437A 0.18315
409A -> 437A 0.26198
411A -> 437A 0.48547
412A -> 437A -0.12856
418A -> 438A 0.11854
393B -> 437B 0.11181
398B -> 437B 0.10088
405B -> 437B 0.21414
407B -> 437B 0.10152
408B -> 437B -0.18315
409B -> 437B -0.26198
411B -> 437B -0.48547
412B -> 437B 0.12856
418B -> 438B -0.11854

Excited State 153: 1.000-A 2.5527 eV 485.70 nm f=0.0036 <S**2>=0.000
401A -> 437A 0.15460
402A -> 437A -0.14324
405A -> 437A -0.11294
408A -> 437A -0.12252
409A -> 438A 0.11139
410A -> 437A 0.36603
411A -> 437A 0.16609
414A -> 437A 0.23299
414A -> 438A -0.10319

415A -> 437A -0.10974
417A -> 438A 0.22843
418A -> 438A 0.24079
401B -> 437B 0.15460
402B -> 437B -0.14324
405B -> 437B -0.11294
408B -> 437B -0.12252
409B -> 438B 0.11139
410B -> 437B 0.36603
411B -> 437B 0.16609
414B -> 437B 0.23299
414B -> 438B -0.10319
415B -> 437B -0.10974
417B -> 438B 0.22843
418B -> 438B 0.24079

Excited State 154: 1.000-A 2.5605 eV 484.23 nm f=0.0058 <S**2>=0.000
408A -> 439A -0.17661
410A -> 439A -0.19753
414A -> 439A -0.13853
415A -> 439A -0.19762
416A -> 439A 0.57950
408B -> 439B -0.17661
410B -> 439B -0.19753
414B -> 439B -0.13853
415B -> 439B -0.19762
416B -> 439B 0.57950

Excited State 155: 3.000-A 2.5611 eV 484.10 nm f=0.0000 <S**2>=2.000
395A -> 438A 0.10368
406A -> 438A -0.14183
408A -> 438A 0.17691
409A -> 437A -0.15697
409A -> 438A -0.15861
411A -> 437A -0.15367
413A -> 438A 0.19331

414A -> 437A -0.11239
415A -> 438A -0.22060
417A -> 437A -0.12185
417A -> 438A 0.27793
418A -> 437A -0.14397
418A -> 438A 0.25835
395B -> 438B -0.10368
406B -> 438B 0.14183
408B -> 438B -0.17691
409B -> 437B 0.15697
409B -> 438B 0.15861
411B -> 437B 0.15367
413B -> 438B -0.19331
414B -> 437B 0.11239
415B -> 438B 0.22060
417B -> 437B 0.12185
417B -> 438B -0.27793
418B -> 437B 0.14397
418B -> 438B -0.25835

Excited State 156: 3.000-A 2.5706 eV 482.31 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.16051
408A -> 437A -0.17761
409A -> 437A 0.21579
410A -> 437A 0.28819
412A -> 437A 0.16385
414A -> 438A 0.12997
415A -> 438A 0.10431
417A -> 437A -0.13306
417A -> 438A 0.27335
418A -> 438A 0.28143
393B -> 437B -0.16051
408B -> 437B 0.17761
409B -> 437B -0.21579
410B -> 437B -0.28819
412B -> 437B -0.16385

414B -> 438B -0.12997
415B -> 438B -0.10431
417B -> 437B 0.13306
417B -> 438B -0.27335
418B -> 438B -0.28143

Excited State 157: 3.000-A 2.5718 eV 482.10 nm f=0.0000 <S**2>=2.000
430A -> 440A -0.19082
433A -> 440A -0.62308
434A -> 440A -0.10801
435A -> 440A 0.15063
436A -> 440A -0.16977
430B -> 440B 0.19082
433B -> 440B 0.62308
434B -> 440B 0.10801
435B -> 440B -0.15063
436B -> 440B 0.16977

Excited State 158: 1.000-A 2.5727 eV 481.92 nm f=0.0025 <S**2>=0.000
402A -> 437A 0.12296
408A -> 437A 0.10479
408A -> 438A 0.10899
409A -> 437A 0.39557
409A -> 438A -0.11275
414A -> 437A -0.11622
414A -> 438A 0.24604
416A -> 438A 0.11099
417A -> 437A -0.10490
417A -> 438A 0.20079
418A -> 438A 0.26619
402B -> 437B 0.12296
408B -> 437B 0.10479
408B -> 438B 0.10899
409B -> 437B 0.39557
409B -> 438B -0.11275
414B -> 437B -0.11622

414B -> 438B 0.24604
416B -> 438B 0.11099
417B -> 437B -0.10490
417B -> 438B 0.20079
418B -> 438B 0.26619

Excited State 159: 1.000-A 2.5772 eV 481.08 nm f=0.0086 <S**2>=0.000
405A -> 437A -0.16312
409A -> 437A 0.37555
409A -> 438A -0.13741
411A -> 437A 0.28360
413A -> 438A 0.10513
414A -> 438A -0.19272
415A -> 438A -0.10342
416A -> 438A -0.15287
417A -> 438A -0.13672
418A -> 438A -0.25800
405B -> 437B -0.16312
409B -> 437B 0.37555
409B -> 438B -0.13741
411B -> 437B 0.28360
413B -> 438B 0.10513
414B -> 438B -0.19272
415B -> 438B -0.10342
416B -> 438B -0.15287
417B -> 438B -0.13672
418B -> 438B -0.25800

Excited State 160: 3.000-A 2.5831 eV 479.99 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.10872
408A -> 437A -0.11183
409A -> 438A -0.18540
410A -> 437A 0.28950
413A -> 437A 0.12000
413A -> 438A 0.22288
414A -> 437A 0.12849

414A -> 438A -0.10135
415A -> 437A -0.11392
415A -> 438A -0.27280
416A -> 438A -0.13453
418A -> 438A -0.24790
393B -> 437B -0.10872
408B -> 437B 0.11183
409B -> 438B 0.18540
410B -> 437B -0.28950
413B -> 437B -0.12000
413B -> 438B -0.22288
414B -> 437B -0.12849
414B -> 438B 0.10135
415B -> 437B 0.11392
415B -> 438B 0.27280
416B -> 438B 0.13453
418B -> 438B 0.24790

Excited State 161: 1.000-A 2.5840 eV 479.81 nm f=0.0004 <S**2>=0.000
430A -> 440A 0.17053
433A -> 440A 0.63565
434A -> 440A 0.13250
435A -> 440A -0.14344
436A -> 440A 0.15319
430B -> 440B 0.17053
433B -> 440B 0.63565
434B -> 440B 0.13250
435B -> 440B -0.14344
436B -> 440B 0.15319

Excited State 162: 3.000-A 2.5948 eV 477.82 nm f=0.0000 <S**2>=2.000
396A -> 439A -0.16047
406A -> 439A 0.11635
407A -> 439A -0.20736
409A -> 439A -0.26826
414A -> 439A 0.32721

416A -> 439A -0.40870
419A -> 439A -0.15348
396B -> 439B 0.16047
406B -> 439B -0.11635
407B -> 439B 0.20736
409B -> 439B 0.26826
414B -> 439B -0.32721
416B -> 439B 0.40870
419B -> 439B 0.15348

Excited State 163: 1.000-A 2.5990 eV 477.05 nm f=0.0237 <S**2>=0.000
408A -> 439A -0.10847
411A -> 439A 0.11999
414A -> 439A 0.59577
416A -> 439A 0.13522
436A -> 444A -0.14166
408B -> 439B -0.10847
411B -> 439B 0.11999
414B -> 439B 0.59577
416B -> 439B 0.13522
436B -> 444B -0.14166

Excited State 164: 1.000-A 2.6041 eV 476.11 nm f=0.0006 <S**2>=0.000
397A -> 437A -0.10905
398A -> 437A 0.28721
400A -> 437A 0.10085
401A -> 437A -0.28804
402A -> 437A 0.17200
407A -> 437A -0.17448
410A -> 437A 0.34987
411A -> 437A -0.11893
412A -> 437A 0.14066
413A -> 437A 0.10520
418A -> 438A -0.10894
397B -> 437B -0.10905
398B -> 437B 0.28721

400B -> 437B 0.10085
401B -> 437B -0.28804
402B -> 437B 0.17200
407B -> 437B -0.17448
410B -> 437B 0.34987
411B -> 437B -0.11893
412B -> 437B 0.14066
413B -> 437B 0.10520
418B -> 438B -0.10894

Excited State 165: 3.000-A 2.6163 eV 473.90 nm f=0.0000 <S**2>=2.000
433A -> 440A -0.12570
434A -> 440A 0.66446
435A -> 440A -0.15586
433B -> 440B 0.12570
434B -> 440B -0.66446
435B -> 440B 0.15586

Excited State 166: 1.000-A 2.6163 eV 473.89 nm f=0.0000 <S**2>=0.000
433A -> 440A -0.14875
434A -> 440A 0.66174
435A -> 440A -0.15345
433B -> 440B -0.14875
434B -> 440B 0.66174
435B -> 440B -0.15345

Excited State 167: 1.000-A 2.6337 eV 470.76 nm f=0.0056 <S**2>=0.000
402A -> 437A 0.11594
405A -> 438A -0.15759
406A -> 438A 0.14244
407A -> 437A 0.23288
407A -> 438A 0.18097
408A -> 437A -0.21831
408A -> 438A -0.12562
413A -> 438A -0.19813
414A -> 438A -0.24487

415A -> 438A 0.34761
402B -> 437B 0.11594
405B -> 438B -0.15759
406B -> 438B 0.14244
407B -> 437B 0.23288
407B -> 438B 0.18097
408B -> 437B -0.21831
408B -> 438B -0.12562
413B -> 438B -0.19813
414B -> 438B -0.24487
415B -> 438B 0.34761

Excited State 168: 1.000-A 2.6439 eV 468.95 nm f=0.0093 <S**2>=0.000
393A -> 437A 0.10984
402A -> 437A 0.16016
405A -> 437A 0.34402
406A -> 437A -0.14307
407A -> 437A 0.26245
408A -> 437A -0.21238
414A -> 438A 0.16777
415A -> 438A -0.23417
393B -> 437B 0.10984
402B -> 437B 0.16016
405B -> 437B 0.34402
406B -> 437B -0.14307
407B -> 437B 0.26245
408B -> 437B -0.21238
414B -> 438B 0.16777
415B -> 438B -0.23417

Excited State 169: 3.000-A 2.6456 eV 468.64 nm f=0.0000 <S**2>=2.000
400A -> 438A 0.11640
406A -> 437A 0.12023
407A -> 438A 0.12941
408A -> 437A 0.17445
408A -> 438A -0.10483

409A -> 438A 0.12297
410A -> 437A 0.10045
410A -> 438A 0.30522
414A -> 438A 0.35295
415A -> 438A -0.27850
400B -> 438B -0.11640
406B -> 437B -0.12023
407B -> 438B -0.12941
408B -> 437B -0.17445
408B -> 438B 0.10483
409B -> 438B -0.12297
410B -> 437B -0.10045
410B -> 438B -0.30522
414B -> 438B -0.35295
415B -> 438B 0.27850

Excited State 170: 3.000-A 2.6479 eV 468.23 nm f=0.0000 <S**2>=2.000
397A -> 437A -0.11021
402A -> 437A -0.15159
405A -> 437A 0.32122
406A -> 437A 0.14513
407A -> 437A 0.36165
409A -> 437A 0.17517
410A -> 437A -0.17838
415A -> 438A -0.13629
397B -> 437B 0.11021
402B -> 437B 0.15159
405B -> 437B -0.32122
406B -> 437B -0.14513
407B -> 437B -0.36165
409B -> 437B -0.17517
410B -> 437B 0.17838
415B -> 438B 0.13629

Excited State 171: 1.000-A 2.6517 eV 467.57 nm f=0.0164 <S**2>=0.000
395A -> 438A 0.10719

401A -> 437A 0.11772
405A -> 437A 0.26759
406A -> 437A 0.16697
407A -> 437A 0.16065
408A -> 437A 0.29288
408A -> 438A 0.13907
410A -> 437A 0.15228
410A -> 438A 0.30515
417A -> 438A -0.12903
395B -> 438B 0.10719
401B -> 437B 0.11772
405B -> 437B 0.26759
406B -> 437B 0.16697
407B -> 437B 0.16065
408B -> 437B 0.29288
408B -> 438B 0.13907
410B -> 437B 0.15228
410B -> 438B 0.30515
417B -> 438B -0.12903

Excited State 172: 3.000-A 2.6574 eV 466.57 nm f=0.0000 <S**2>=2.000
430A -> 441A 0.10886
430A -> 442A 0.20234
433A -> 441A 0.18317
433A -> 442A 0.30729
435A -> 442A 0.15936
436A -> 441A -0.20195
436A -> 442A -0.32480
430B -> 441B -0.10886
430B -> 442B -0.20234
433B -> 441B -0.18317
433B -> 442B -0.30729
435B -> 442B -0.15936
436B -> 441B 0.20195
436B -> 442B 0.32480

Excited State 173: 3.000-A 2.6668 eV 464.91 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 401A -> 439A | -0.12960 |
| 408A -> 439A | -0.16532 |
| 409A -> 439A | 0.11974 |
| 410A -> 439A | 0.25478 |
| 411A -> 439A | 0.26458 |
| 413A -> 439A | 0.22916 |
| 414A -> 439A | -0.23081 |
| 415A -> 439A | -0.32187 |
| 416A -> 439A | -0.15787 |
| 401B -> 439B | 0.12960 |
| 408B -> 439B | 0.16532 |
| 409B -> 439B | -0.11974 |
| 410B -> 439B | -0.25478 |
| 411B -> 439B | -0.26458 |
| 413B -> 439B | -0.22916 |
| 414B -> 439B | 0.23081 |
| 415B -> 439B | 0.32187 |
| 416B -> 439B | 0.15787 |

Excited State 174: 1.000-A 2.6698 eV 464.39 nm f=0.0080 <S**2>=0.000

| | |
|---|---|
| 401A -> 437A | -0.15084 |
| 402A -> 437A | -0.24739 |
| 405A -> 437A | 0.14208 |
| 406A -> 437A | 0.48888 |
| 406A -> 438A | -0.10249 |
| 408A -> 438A | -0.17252 |
| 415A -> 438A | -0.10358 |
| 401B -> 437B | -0.15084 |
| 402B -> 437B | -0.24739 |
| 405B -> 437B | 0.14208 |
| 406B -> 437B | 0.48888 |
| 406B -> 438B | -0.10249 |
| 408B -> 438B | -0.17252 |
| 415B -> 438B | -0.10358 |

Excited State 175: 3.000-A 2.6702 eV 464.32 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 397A -> 437A | 0.10359 |
| 405A -> 437A | 0.16901 |
| 406A -> 437A | 0.42207 |
| 406A -> 438A | -0.14940 |
| 408A -> 437A | 0.28247 |
| 410A -> 437A | 0.19518 |
| 414A -> 438A | -0.17317 |
| 415A -> 438A | 0.18464 |
| 397B -> 437B | -0.10359 |
| 405B -> 437B | -0.16901 |
| 406B -> 437B | -0.42207 |
| 406B -> 438B | 0.14940 |
| 408B -> 437B | -0.28247 |
| 410B -> 437B | -0.19518 |
| 414B -> 438B | 0.17317 |
| 415B -> 438B | -0.18464 |

Excited State 176: 1.000-A 2.6854 eV 461.70 nm f=0.0108 <S**2>=0.000

| | |
|---|---|
| 405A -> 437A | -0.12264 |
| 407A -> 438A | 0.13368 |
| 407A -> 439A | 0.13357 |
| 409A -> 438A | 0.14826 |
| 409A -> 439A | 0.38043 |
| 410A -> 438A | 0.17250 |
| 411A -> 439A | 0.12877 |
| 413A -> 438A | -0.10404 |
| 413A -> 439A | -0.19527 |
| 414A -> 439A | -0.17359 |
| 415A -> 438A | -0.12936 |
| 415A -> 439A | 0.18608 |
| 416A -> 439A | 0.11684 |
| 419A -> 439A | 0.10351 |
| 405B -> 437B | -0.12264 |
| 407B -> 438B | 0.13368 |
| 407B -> 439B | 0.13357 |

409B -> 438B 0.14826
409B -> 439B 0.38043
410B -> 438B 0.17250
411B -> 439B 0.12877
413B -> 438B -0.10404
413B -> 439B -0.19527
414B -> 439B -0.17359
415B -> 438B -0.12936
415B -> 439B 0.18608
416B -> 439B 0.11684
419B -> 439B 0.10351

Excited State 177: 3.000-A 2.6855 eV 461.68 nm f=0.0000 <S**2>=2.000
406A -> 437A -0.29027
407A -> 437A 0.21118
408A -> 437A 0.32101
408A -> 438A 0.24149
410A -> 437A 0.14829
410A -> 438A 0.19240
411A -> 438A -0.14526
417A -> 438A -0.12983
406B -> 437B 0.29027
407B -> 437B -0.21118
408B -> 437B -0.32101
408B -> 438B -0.24149
410B -> 437B -0.14829
410B -> 438B -0.19240
411B -> 438B 0.14526
417B -> 438B 0.12983

Excited State 178: 1.000-A 2.6895 eV 460.99 nm f=0.0270 <S**2>=0.000
405A -> 437A 0.16400
407A -> 438A -0.20523
408A -> 438A 0.10780
409A -> 438A -0.21867
409A -> 439A 0.25272

410A -> 438A -0.23681
412A -> 438A -0.15052
413A -> 438A 0.17970
413A -> 439A -0.13433
415A -> 438A 0.23668
415A -> 439A 0.11228
405B -> 437B 0.16400
407B -> 438B -0.20523
408B -> 438B 0.10780
409B -> 438B -0.21867
409B -> 439B 0.25272
410B -> 438B -0.23681
412B -> 438B -0.15052
413B -> 438B 0.17970
413B -> 439B -0.13433
415B -> 438B 0.23668
415B -> 439B 0.11228

Excited State 179: 3.000-A 2.7066 eV 458.08 nm f=0.0000 <S**2>=2.000
400A -> 438A -0.10634
409A -> 438A 0.12968
410A -> 438A -0.28896
411A -> 438A -0.28547
412A -> 438A 0.16749
413A -> 438A -0.28643
415A -> 438A -0.28135
416A -> 438A -0.19167
400B -> 438B 0.10634
409B -> 438B -0.12968
410B -> 438B 0.28896
411B -> 438B 0.28547
412B -> 438B -0.16749
413B -> 438B 0.28643
415B -> 438B 0.28135
416B -> 438B 0.19167

Excited State 180: 1.000-A 2.7097 eV 457.56 nm f=0.0034 <S**2>=0.000

| | |
|---|---|
| 408A -> 437A | -0.12072 |
| 408A -> 439A | -0.11730 |
| 409A -> 439A | 0.12965 |
| 410A -> 439A | 0.15776 |
| 411A -> 439A | 0.37955 |
| 412A -> 439A | -0.12420 |
| 413A -> 439A | 0.23408 |
| 415A -> 439A | -0.32092 |
| 416A -> 439A | -0.10187 |
| 408B -> 437B | -0.12072 |
| 408B -> 439B | -0.11730 |
| 409B -> 439B | 0.12965 |
| 410B -> 439B | 0.15776 |
| 411B -> 439B | 0.37955 |
| 412B -> 439B | -0.12420 |
| 413B -> 439B | 0.23408 |
| 415B -> 439B | -0.32092 |
| 416B -> 439B | -0.10187 |

Excited State 181: 1.000-A 2.7114 eV 457.27 nm f=0.0085 <S**2>=0.000

| | |
|---|---|
| 395A -> 438A | -0.12924 |
| 403A -> 437A | 0.16220 |
| 403A -> 438A | 0.14117 |
| 406A -> 438A | -0.19441 |
| 407A -> 437A | 0.12829 |
| 407A -> 438A | 0.22723 |
| 408A -> 437A | 0.32183 |
| 410A -> 437A | 0.18437 |
| 410A -> 438A | -0.17483 |
| 411A -> 439A | 0.16064 |
| 415A -> 439A | -0.12969 |
| 395B -> 438B | -0.12924 |
| 403B -> 437B | 0.16220 |
| 403B -> 438B | 0.14117 |
| 406B -> 438B | -0.19441 |

407B -> 437B 0.12829
407B -> 438B 0.22723
408B -> 437B 0.32183
410B -> 437B 0.18437
410B -> 438B -0.17483
411B -> 439B 0.16064
415B -> 439B -0.12969

Excited State 182: 1.000-A 2.7199 eV 455.85 nm f=0.0036 <S**2>=0.000
407A -> 438A 0.11814
410A -> 438A 0.30368
411A -> 438A 0.37858
412A -> 438A -0.17072
413A -> 438A 0.27910
415A -> 438A 0.20341
416A -> 438A 0.12642
407B -> 438B 0.11814
410B -> 438B 0.30368
411B -> 438B 0.37858
412B -> 438B -0.17072
413B -> 438B 0.27910
415B -> 438B 0.20341
416B -> 438B 0.12642

Excited State 183: 3.000-A 2.7225 eV 455.40 nm f=0.0000 <S**2>=2.000
403A -> 437A 0.15085
409A -> 438A 0.23333
410A -> 438A -0.12127
411A -> 438A -0.27097
412A -> 438A -0.11157
413A -> 438A 0.38893
415A -> 438A 0.15278
434A -> 441A -0.11506
435A -> 441A -0.15717
435A -> 443A 0.13559
403B -> 437B -0.15085

409B -> 438B -0.23333
410B -> 438B 0.12127
411B -> 438B 0.27097
412B -> 438B 0.11157
413B -> 438B -0.38893
415B -> 438B -0.15278
434B -> 441B 0.11506
435B -> 441B 0.15717
435B -> 443B -0.13559

Excited State 184: 1.000-A 2.7228 eV 455.35 nm f=0.0171 <S**2>=0.000
397A -> 437A -0.11222
398A -> 437A 0.17652
402A -> 437A -0.27681
403A -> 437A -0.23022
406A -> 437A -0.17330
407A -> 437A 0.30460
408A -> 438A 0.19627
411A -> 438A -0.20717
413A -> 438A 0.15475
397B -> 437B -0.11222
398B -> 437B 0.17652
402B -> 437B -0.27681
403B -> 437B -0.23022
406B -> 437B -0.17330
407B -> 437B 0.30460
408B -> 438B 0.19627
411B -> 438B -0.20717
413B -> 438B 0.15475

Excited State 185: 3.000-A 2.7245 eV 455.07 nm f=0.0000 <S**2>=2.000
411A -> 438A 0.17428
413A -> 438A -0.13062
434A -> 441A -0.26815
434A -> 442A 0.10916
435A -> 441A -0.43243

435A -> 442A 0.16900
436A -> 441A -0.20412
411B -> 438B -0.17428
413B -> 438B 0.13062
434B -> 441B 0.26815
434B -> 442B -0.10916
435B -> 441B 0.43243
435B -> 442B -0.16900
436B -> 441B 0.20412

Excited State 186: 3.000-A 2.7297 eV 454.21 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.24534
403A -> 437A 0.47000
405A -> 437A 0.28342
407A -> 437A -0.15727
409A -> 437A 0.12079
413A -> 438A -0.13916
400B -> 437B 0.24534
403B -> 437B -0.47000
405B -> 437B -0.28342
407B -> 437B 0.15727
409B -> 437B -0.12079
413B -> 438B 0.13916

Excited State 187: 1.000-A 2.7349 eV 453.34 nm f=0.0067 <S**2>=0.000
402A -> 437A 0.13109
408A -> 438A -0.13029
409A -> 438A 0.31933
411A -> 438A -0.33248
413A -> 438A 0.37034
415A -> 438A 0.10133
402B -> 437B 0.13109
408B -> 438B -0.13029
409B -> 438B 0.31933
411B -> 438B -0.33248
413B -> 438B 0.37034

415B -> 438B 0.10133

Excited State 188: 3.000-A 2.7363 eV 453.11 nm f=0.0000 <S**2>=2.000
408A -> 439A -0.31082
409A -> 439A 0.10297
410A -> 439A 0.18558
411A -> 439A -0.43555
412A -> 439A 0.23916
413A -> 439A -0.20974
415A -> 439A -0.10705
416A -> 439A -0.10348
408B -> 439B 0.31082
409B -> 439B -0.10297
410B -> 439B -0.18558
411B -> 439B 0.43555
412B -> 439B -0.23916
413B -> 439B 0.20974
415B -> 439B 0.10705
416B -> 439B 0.10348

Excited State 189: 3.000-A 2.7454 eV 451.61 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.10499
400A -> 438A 0.17436
403A -> 437A 0.12401
406A -> 437A 0.15291
408A -> 437A -0.15601
409A -> 438A -0.20978
410A -> 438A 0.11802
411A -> 438A -0.36537
412A -> 438A 0.15169
434A -> 443A 0.15833
435A -> 443A -0.23939
436A -> 443A -0.12248
400B -> 437B -0.10499
400B -> 438B -0.17436
403B -> 437B -0.12401

406B -> 437B -0.15291
408B -> 437B 0.15601
409B -> 438B 0.20978
410B -> 438B -0.11802
411B -> 438B 0.36537
412B -> 438B -0.15169
434B -> 443B -0.15833
435B -> 443B 0.23939
436B -> 443B 0.12248

Excited State 190: 1.000-A 2.7459 eV 451.53 nm f=0.0044 <S**2>=0.000
400A -> 437A -0.24631
402A -> 437A -0.10484
403A -> 437A 0.42867
405A -> 437A 0.21510
408A -> 437A -0.16344
408A -> 438A 0.15469
410A -> 438A 0.11551
411A -> 438A -0.14434
400B -> 437B -0.24631
402B -> 437B -0.10484
403B -> 437B 0.42867
405B -> 437B 0.21510
408B -> 437B -0.16344
408B -> 438B 0.15469
410B -> 438B 0.11551
411B -> 438B -0.14434

Excited State 191: 1.000-A 2.7507 eV 450.73 nm f=0.0029 <S**2>=0.000
408A -> 439A 0.37809
409A -> 439A -0.15923
410A -> 439A -0.16387
411A -> 439A 0.33573
412A -> 439A -0.21706
413A -> 439A 0.17283
415A -> 439A 0.24414

416A -> 439A 0.12788
408B -> 439B 0.37809
409B -> 439B -0.15923
410B -> 439B -0.16387
411B -> 439B 0.33573
412B -> 439B -0.21706
413B -> 439B 0.17283
415B -> 439B 0.24414
416B -> 439B 0.12788

Excited State 192: 3.000-A 2.7570 eV 449.71 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.12312
400A -> 438A 0.16183
404A -> 437A 0.25171
406A -> 438A 0.11030
407A -> 438A -0.12496
408A -> 437A 0.18899
408A -> 438A -0.22507
409A -> 438A -0.27217
434A -> 443A -0.14964
435A -> 443A 0.23966
436A -> 443A 0.14330
400B -> 437B -0.12312
400B -> 438B -0.16183
404B -> 437B -0.25171
406B -> 438B -0.11030
407B -> 438B 0.12496
408B -> 437B -0.18899
408B -> 438B 0.22507
409B -> 438B 0.27217
434B -> 443B 0.14964
435B -> 443B -0.23966
436B -> 443B -0.14330

Excited State 193: 3.000-A 2.7590 eV 449.38 nm f=0.0000 <S**2>=2.000
399A -> 437A 0.10963

400A -> 437A 0.12856
402A -> 437A 0.15424
403A -> 437A 0.31545
404A -> 437A 0.21969
405A -> 437A -0.27125
406A -> 437A 0.25200
406A -> 438A -0.10668
407A -> 437A 0.16835
408A -> 438A 0.13072
410A -> 438A 0.10774
411A -> 438A 0.13183
399B -> 437B -0.10963
400B -> 437B -0.12856
402B -> 437B -0.15424
403B -> 437B -0.31545
404B -> 437B -0.21969
405B -> 437B 0.27125
406B -> 437B -0.25200
406B -> 438B 0.10668
407B -> 437B -0.16835
408B -> 438B -0.13072
410B -> 438B -0.10774
411B -> 438B -0.13183

Excited State 194: 3.000-A 2.7639 eV 448.58 nm f=0.0000 <S**2>=2.000
404A -> 437A -0.13539
407A -> 439A -0.33442
408A -> 438A 0.11442
409A -> 439A 0.14003
410A -> 438A 0.11540
410A -> 439A 0.18594
413A -> 439A -0.13026
415A -> 439A 0.23114
435A -> 443A 0.10286
436A -> 443A 0.11511
436A -> 444A -0.23259

404B -> 437B 0.13539
407B -> 439B 0.33442
408B -> 438B -0.11442
409B -> 439B -0.14003
410B -> 438B -0.11540
410B -> 439B -0.18594
413B -> 439B 0.13026
415B -> 439B -0.23114
435B -> 443B -0.10286
436B -> 443B -0.11511
436B -> 444B 0.23259

Excited State 195: 3.000-A 2.7650 eV 448.41 nm f=0.0000 <S**2>=2.000
404A -> 437A 0.10671
407A -> 439A -0.25244
408A -> 437A 0.13101
408A -> 438A -0.15094
409A -> 438A 0.10064
410A -> 438A -0.14360
410A -> 439A 0.14888
415A -> 439A 0.21135
434A -> 443A 0.11749
435A -> 443A -0.18342
436A -> 443A -0.15987
436A -> 444A 0.22070
404B -> 437B -0.10671
407B -> 439B 0.25244
408B -> 437B -0.13101
408B -> 438B 0.15094
409B -> 438B -0.10064
410B -> 438B 0.14360
410B -> 439B -0.14888
415B -> 439B -0.21135
434B -> 443B -0.11749
435B -> 443B 0.18342
436B -> 443B 0.15987

436B -> 444B -0.22070

Excited State 196: 1.000-A 2.7655 eV 448.32 nm f=0.0009 <S**2>=0.000
400A -> 437A 0.21376
402A -> 437A 0.16735
402A -> 438A -0.10566
403A -> 437A 0.22383
404A -> 437A 0.22701
405A -> 437A -0.22003
405A -> 438A 0.10983
406A -> 437A 0.25588
406A -> 438A -0.14888
407A -> 437A 0.13230
408A -> 437A -0.12242
408A -> 438A 0.14753
410A -> 437A -0.10134
410A -> 438A 0.19608
400B -> 437B 0.21376
402B -> 437B 0.16735
402B -> 438B -0.10566
403B -> 437B 0.22383
404B -> 437B 0.22701
405B -> 437B -0.22003
405B -> 438B 0.10983
406B -> 437B 0.25588
406B -> 438B -0.14888
407B -> 437B 0.13230
408B -> 437B -0.12242
408B -> 438B 0.14753
410B -> 437B -0.10134
410B -> 438B 0.19608

Excited State 197: 3.000-A 2.7691 eV 447.75 nm f=0.0000 <S**2>=2.000
404A -> 437A 0.15900
408A -> 438A -0.11048
410A -> 438A -0.11570

433A -> 444A -0.12652
434A -> 443A 0.11334
435A -> 443A -0.22592
435A -> 444A 0.15071
436A -> 442A 0.13110
436A -> 444A -0.44771
404B -> 437B -0.15900
408B -> 438B 0.11048
410B -> 438B 0.11570
433B -> 444B 0.12652
434B -> 443B -0.11334
435B -> 443B 0.22592
435B -> 444B -0.15071
436B -> 442B -0.13110
436B -> 444B 0.44771

Excited State 198: 1.000-A 2.7765 eV 446.55 nm f=0.0016 <S**2>=0.000
400A -> 438A 0.10235
402A -> 437A -0.12986
403A -> 437A -0.13859
404A -> 437A 0.42501
405A -> 437A 0.17877
407A -> 437A -0.17250
408A -> 438A -0.22208
409A -> 438A -0.18887
410A -> 438A 0.10845
411A -> 438A -0.16191
412A -> 438A 0.17771
400B -> 438B 0.10235
402B -> 437B -0.12986
403B -> 437B -0.13859
404B -> 437B 0.42501
405B -> 437B 0.17877
407B -> 437B -0.17250
408B -> 438B -0.22208
409B -> 438B -0.18887

410B -> 438B 0.10845
411B -> 438B -0.16191
412B -> 438B 0.17771

Excited State 199: 1.000-A 2.7816 eV 445.73 nm f=0.0016 <S**2>=0.000
397A -> 437A -0.17231
398A -> 437A 0.11402
400A -> 437A -0.16051
403A -> 437A 0.17614
403A -> 438A -0.16543
404A -> 437A 0.41436
404A -> 438A -0.12321
406A -> 438A 0.12567
407A -> 437A 0.15463
407A -> 438A -0.13839
408A -> 437A 0.11663
410A -> 438A -0.16386
411A -> 438A 0.10676
412A -> 438A -0.13102
397B -> 437B -0.17231
398B -> 437B 0.11402
400B -> 437B -0.16051
403B -> 437B 0.17614
403B -> 438B -0.16543
404B -> 437B 0.41436
404B -> 438B -0.12321
406B -> 438B 0.12567
407B -> 437B 0.15463
407B -> 438B -0.13839
408B -> 437B 0.11663
410B -> 438B -0.16386
411B -> 438B 0.10676
412B -> 438B -0.13102

Excited State 200: 3.000-A 2.7818 eV 445.70 nm f=0.0000 <S**2>=2.000
403A -> 437A -0.18555

| | |
|---|---|
| 404A -> 437A | 0.51835 |
| 405A -> 437A | 0.17266 |
| 407A -> 437A | -0.19730 |
| 407A -> 438A | 0.14269 |
| 408A -> 437A | -0.14351 |
| 408A -> 438A | 0.14538 |
| 403B -> 437B | 0.18555 |
| 404B -> 437B | -0.51835 |
| 405B -> 437B | -0.17266 |
| 407B -> 437B | 0.19730 |
| 407B -> 438B | -0.14269 |
| 408B -> 437B | 0.14351 |
| 408B -> 438B | -0.14538 |

**Table S13.** Standard orientation of the optimized geometry for the open-ring isomer (OF6) of **[Ir(μ-Cl)(PIC)$_2$]$_2$**.

| Symbol | Coordinates | | |
|---|---|---|---|
| | X | Y | Z |
| Ir | -0.153771 | -2.250449 | -0.057884 |
| N | 4.103067 | -3.237218 | -0.767133 |
| C | 3.210558 | -2.546683 | 0.036781 |
| C | 3.661157 | -2.070047 | 1.309387 |
| C | 5.073526 | -2.136334 | 1.669897 |
| C | 6.166387 | -2.184958 | 0.736725 |
| C | 6.174008 | -1.427638 | -0.491215 |
| C | 7.265017 | -1.410786 | -1.310423 |
| C | 8.46192 | -2.189438 | -1.01314 |
| C | 8.44201 | -2.953099 | 0.236478 |
| C | 7.364414 | -2.918347 | 1.072028 |
| O | 9.470215 | -2.200232 | -1.780068 |
| C | 2.7296 | -1.758983 | 2.333904 |
| C | 3.108579 | -1.636052 | 3.654667 |
| C | 4.45809 | -1.835381 | 4.03012 |
| C | 5.405296 | -2.090932 | 3.060429 |
| C | 3.428645 | -3.726436 | -1.815049 |
| C | 2.038848 | -3.337403 | -1.675107 |
| N | 1.910685 | -2.618824 | -0.507195 |
| C | 4.112381 | -4.602345 | -2.778107 |
| C | 0.840691 | -3.706733 | -2.365682 |
| C | 0.788307 | -4.287827 | -3.655012 |
| C | -0.422798 | -4.73604 | -4.165437 |
| C | -1.591322 | -4.618879 | -3.389548 |
| C | -1.558214 | -3.996238 | -2.140107 |
| C | -0.359994 | -3.474363 | -1.620024 |
| C | 5.411674 | -4.25716 | -3.205814 |
| C | 6.124862 | -5.094765 | -4.065733 |
| C | 5.560099 | -6.298614 | -4.504587 |
| C | 4.279862 | -6.663073 | -4.06926 |
| C | 3.560934 | -5.825396 | -3.212988 |
| N | 4.360135 | 2.022627 | 1.062012 |
| C | 3.420617 | 1.845633 | 0.049011 |
| C | 3.895896 | 1.567836 | -1.281254 |
| C | 5.233993 | 1.984636 | -1.627914 |
| C | 5.969463 | 2.980303 | -0.875587 |
| C | 5.346786 | 4.192962 | -0.401409 |
| C | 6.072185 | 5.19313 | 0.174716 |
| C | 7.514156 | 5.070667 | 0.369898 |
| C | 8.135629 | 3.838654 | -0.124715 |
| C | 7.400334 | 2.868247 | -0.741062 |
| O | 8.200784 | 5.98165 | 0.918522 |
| C | 3.153066 | 0.819423 | -2.222614 |
| C | 3.726508 | 0.400579 | -3.412369 |
| C | 5.069427 | 0.719394 | -3.713263 |
| C | 5.810407 | 1.484801 | -2.828738 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.71219 | 2.529627 | 2.124256 | C | -5.194882 | -5.22426 | 4.731153 |
| C | 2.308713 | 2.632426 | 1.790602 | C | -4.39325 | -4.753439 | 3.686923 |
| N | 2.140778 | 2.115203 | 0.511625 | N | -4.169798 | 2.773837 | -1.040353 |
| C | 4.453857 | 2.846172 | 3.35838 | C | -3.261556 | 2.338062 | -0.084283 |
| C | 1.16274 | 3.252216 | 2.383679 | C | -3.75616 | 1.993887 | 1.217585 |
| C | 1.111895 | 3.837507 | 3.671639 | C | -3.055508 | 1.135156 | 2.094903 |
| C | 0.015313 | 4.603116 | 4.043672 | C | -3.647909 | 0.655308 | 3.249113 |
| C | -1.036216 | 4.812307 | 3.129683 | C | -4.978911 | 1.006118 | 3.572649 |
| C | -1.025657 | 4.190256 | 1.880574 | C | -5.680556 | 1.871884 | 2.754856 |
| C | 0.032119 | 3.344579 | 1.499876 | C | -3.467108 | 3.261565 | -2.075276 |
| C | 5.359 | 1.89906 | 3.875848 | C | -2.059834 | 3.064229 | -1.794933 |
| C | 6.125159 | 2.191647 | 5.006304 | N | -1.955523 | 2.425127 | -0.568821 |
| C | 6.013357 | 3.439585 | 5.631774 | C | -4.1778 | 3.863952 | -3.216139 |
| C | 5.135679 | 4.39743 | 5.111384 | C | -0.837131 | 3.487672 | -2.408987 |
| C | 4.363568 | 4.105639 | 3.983002 | C | -0.714327 | 4.072403 | -3.692063 |
| Cl | -0.004588 | -0.092062 | 1.599552 | C | 0.493517 | 4.62884 | -4.090964 |
| Cl | -0.00759 | -0.076496 | -1.687551 | C | 1.589676 | 4.625023 | -3.207282 |
| Ir | 0.089708 | 2.084928 | -0.040067 | C | 1.497815 | 3.993193 | -1.966537 |
| N | -4.454973 | -2.333651 | 1.016209 | C | 0.313477 | 3.351212 | -1.561423 |
| C | -3.515368 | -2.022052 | 0.040418 | C | -5.366578 | 3.259251 | -3.673885 |
| C | -3.99323 | -1.589516 | -1.242427 | C | -6.108504 | 3.836453 | -4.705779 |
| C | -5.363275 | -1.88605 | -1.603792 | C | -5.689709 | 5.03907 | -5.289531 |
| C | -6.135219 | -2.938881 | -0.985252 | C | -4.529795 | 5.666083 | -4.821349 |
| C | -5.559942 | -4.22901 | -0.680007 | C | -3.781332 | 5.087666 | -3.791801 |
| C | -6.32433 | -5.26996 | -0.244919 | H | 5.306465 | -0.82598 | -0.725966 |
| C | -7.760885 | -5.12183 | -0.030032 | H | 7.282655 | -0.808972 | -2.210642 |
| C | -8.334446 | -3.811399 | -0.351771 | H | 9.317472 | -3.553263 | 0.458765 |
| C | -7.562491 | -2.795515 | -0.834091 | H | 7.367956 | -3.516723 | 1.976171 |
| O | -8.483943 | -6.071428 | 0.390814 | H | 1.693048 | -1.650756 | 2.071808 |
| C | -3.215452 | -0.80988 | -2.127519 | H | 2.360134 | -1.408323 | 4.40532 |
| C | -3.775728 | -0.24382 | -3.259046 | H | 4.75281 | -1.752759 | 5.070835 |
| C | -5.147748 | -0.423943 | -3.548698 | H | 6.448749 | -2.158971 | 3.343922 |
| C | -5.928576 | -1.210782 | -2.722374 | H | 1.691726 | -4.377275 | -4.245056 |
| C | -3.808652 | -2.948601 | 2.01903 | H | -0.466928 | -5.179015 | -5.154719 |
| C | -2.3974 | -2.968971 | 1.698204 | H | -2.533502 | -4.997275 | -3.775406 |
| N | -2.226647 | -2.320716 | 0.481703 | H | -2.47566 | -3.886567 | -1.580418 |
| C | -4.573379 | -3.453588 | 3.173539 | H | 5.848186 | -3.329036 | -2.855838 |
| C | -1.246645 | -3.607969 | 2.262647 | H | 7.120786 | -4.809421 | -4.388827 |
| C | -1.202427 | -4.278619 | 3.50862 | H | 6.114752 | -6.950184 | -5.172215 |
| C | -0.106141 | -5.06538 | 3.835779 | H | 3.84541 | -7.605895 | -4.386105 |
| C | 0.949288 | -5.209291 | 2.915035 | H | 2.584059 | -6.132527 | -2.857789 |
| C | 0.950298 | -4.495209 | 1.715351 | H | 4.281967 | 4.319059 | -0.554351 |
| C | -0.105917 | -3.620196 | 1.391617 | H | 5.610344 | 6.120234 | 0.494444 |
| C | -5.605178 | -2.656078 | 3.708632 | H | 9.203888 | 3.734064 | 0.029416 |
| C | -6.400402 | -3.126917 | 4.755129 | H | 7.879269 | 1.956028 | -1.08029 |
| C | -6.194272 | -4.410573 | 5.276238 | H | 2.145091 | 0.518957 | -1.982932 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.140845 | -0.196457 | -4.102946 | H | -5.049248 | -6.232242 | 5.106157 |
| H | 5.512002 | 0.388332 | -4.646889 | H | -3.650173 | -5.40825 | 3.246617 |
| H | 6.817516 | 1.788941 | -3.091806 | H | -2.065504 | 0.800451 | 1.829753 |
| H | 1.92668 | 3.686283 | 4.367288 | H | -3.092739 | -0.020692 | 3.88999 |
| H | -0.025114 | 5.050767 | 5.031069 | H | -5.437304 | 0.621697 | 4.477642 |
| H | -1.871798 | 5.448226 | 3.407483 | H | -6.671748 | 2.200854 | 3.045754 |
| H | -1.854411 | 4.341297 | 1.202258 | H | -1.560035 | 4.078916 | -4.367028 |
| H | 5.452035 | 0.939733 | 3.38093 | H | 0.58871 | 5.073601 | -5.075883 |
| H | 6.813878 | 1.448748 | 5.39652 | H | 2.521997 | 5.097273 | -3.502785 |
| H | 6.612878 | 3.667867 | 6.50712 | H | 2.361903 | 3.96848 | -1.318594 |
| H | 5.063431 | 5.377169 | 5.572586 | H | -5.698337 | 2.343192 | -3.199978 |
| H | 3.714438 | 4.867493 | 3.565782 | H | -7.018293 | 3.354462 | -5.050029 |
| H | -4.500368 | -4.373315 | -0.853581 | H | -6.26937 | 5.489866 | -6.088511 |
| H | -5.898193 | -6.248533 | -0.055835 | H | -4.215003 | 6.614315 | -5.24517 |
| H | -9.39885 | -3.690276 | -0.183055 | H | -2.908143 | 5.604543 | -3.411114 |
| H | -8.007539 | -1.830382 | -1.051065 | C | -5.069874 | 2.460723 | 1.610772 |
| H | -2.184277 | -0.606558 | -1.886892 | C | -5.730631 | 3.590539 | 1.000456 |
| H | -3.15963 | 0.368409 | -3.908188 | C | -7.168741 | 3.616113 | 0.893993 |
| H | -5.579147 | 0.029202 | -4.434834 | C | -5.016705 | 4.798616 | 0.656483 |
| H | -6.960213 | -1.411605 | -2.988536 | C | -7.829578 | 4.710927 | 0.418962 |
| H | -2.022384 | -4.177761 | 4.207252 | H | -7.718353 | 2.713546 | 1.138796 |
| H | -0.071268 | -5.57969 | 4.790455 | C | -5.665392 | 5.918512 | 0.229524 |
| H | 1.783795 | -5.863571 | 3.149388 | H | -3.943241 | 4.815548 | 0.79825 |
| H | 1.791891 | -4.59983 | 1.043462 | H | -8.905609 | 4.715222 | 0.283841 |
| H | -5.776251 | -1.674409 | 3.283274 | H | -5.132241 | 6.836872 | 0.012008 |
| H | -7.186799 | -2.497173 | 5.159613 | C | -7.115305 | 5.940013 | 0.060288 |
| H | -6.815705 | -4.778019 | 6.086444 | O | -7.733958 | 6.963792 | -0.353396 |

Excited State 1: 3.000-A -0.5908 eV -2098.73 nm f=-0.0000 <S**2>=2.000

434A -> 437A 0.20318

434A -> 438A -0.17995

434A -> 439A -0.24615

434A -> 440A -0.18391

436A -> 437A -0.36927

436A -> 438A 0.27026

436A -> 439A 0.19525

436A -> 440A 0.14964

434B -> 437B -0.20318

434B -> 438B 0.17995

434B -> 439B 0.24615

434B -> 440B 0.18391

436B -> 437B 0.36927
436B -> 438B -0.27026
436B -> 439B -0.19525
436B -> 440B -0.14964
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -6023.89106891
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.000-A -0.5828 eV -2127.29 nm f=-0.0000 <S**2>=2.000
433A -> 438A 0.10007
433A -> 439A -0.28075
433A -> 440A 0.30210
435A -> 437A -0.23435
435A -> 438A -0.33171
435A -> 439A 0.23228
435A -> 440A -0.18628
433B -> 438B -0.10007
433B -> 439B 0.28075
433B -> 440B -0.30210
435B -> 437B 0.23435
435B -> 438B 0.33171
435B -> 439B -0.23228
435B -> 440B 0.18628

Excited State 3: 3.000-A -0.5764 eV -2151.16 nm f=-0.0000 <S**2>=2.000
433A -> 437A -0.18217
433A -> 438A -0.33708
434A -> 437A -0.18858
435A -> 437A -0.14050
435A -> 438A -0.25232
435A -> 439A -0.17676
435A -> 440A 0.32228
436A -> 437A -0.13123
436A -> 439A -0.17198
433B -> 437B 0.18217
433B -> 438B 0.33708

434B -> 437B 0.18858
435B -> 437B 0.14050
435B -> 438B 0.25232
435B -> 439B 0.17676
435B -> 440B -0.32228
436B -> 437B 0.13123
436B -> 439B 0.17198

Excited State 4: 3.000-A -0.5734 eV -2162.26 nm f=-0.0000 <S**2>=2.000
433A -> 437A -0.16921
434A -> 437A 0.26505
434A -> 438A -0.18813
434A -> 439A 0.18245
434A -> 440A 0.15795
435A -> 437A -0.13129
435A -> 439A -0.14924
436A -> 437A 0.22059
436A -> 438A -0.10997
436A -> 439A 0.29002
436A -> 440A 0.26370
433B -> 437B 0.16921
434B -> 437B -0.26505
434B -> 438B 0.18813
434B -> 439B -0.18245
434B -> 440B -0.15795
435B -> 437B 0.13129
435B -> 439B 0.14924
436B -> 437B -0.22059
436B -> 438B 0.10997
436B -> 439B -0.29002
436B -> 440B -0.26370

Excited State 5: 3.000-A 0.6621 eV 1872.62 nm f=0.0000 <S**2>=2.000
435A -> 438A 0.10948
436A -> 437A -0.40308
436A -> 438A -0.54183

435B -> 438B -0.10948
436B -> 437B 0.40308
436B -> 438B 0.54183

Excited State 6: 1.000-A 0.6661 eV 1861.24 nm f=0.0003 <S**2>=0.000
435A -> 437A -0.10145
436A -> 437A 0.40267
436A -> 438A 0.53614
436A -> 439A -0.13194
435B -> 437B -0.10145
436B -> 437B 0.40267
436B -> 438B 0.53614
436B -> 439B -0.13194

Excited State 7: 3.000-A 0.6750 eV 1836.75 nm f=0.0000 <S**2>=2.000
430A -> 439A -0.11401
432A -> 439A 0.13051
433A -> 437A 0.11869
434A -> 437A -0.29259
434A -> 438A 0.18453
435A -> 437A -0.23718
435A -> 438A 0.16544
436A -> 437A -0.12749
436A -> 438A 0.11541
436A -> 439A 0.36465
436A -> 440A 0.21967
430B -> 439B 0.11401
432B -> 439B -0.13051
433B -> 437B -0.11869
434B -> 437B 0.29259
434B -> 438B -0.18453
435B -> 437B 0.23718
435B -> 438B -0.16544
436B -> 437B 0.12749
436B -> 438B -0.11541
436B -> 439B -0.36465

436B -> 440B -0.21967

Excited State 8: 3.000-A 0.6831 eV 1815.00 nm f=0.0000 <S**2>=2.000
434A -> 437A 0.17915
435A -> 437A -0.49315
435A -> 438A 0.29248
436A -> 437A -0.12384
436A -> 438A 0.13605
436A -> 439A -0.23263
434B -> 437B -0.17915
435B -> 437B 0.49315
435B -> 438B -0.29248
436B -> 437B 0.12384
436B -> 438B -0.13605
436B -> 439B 0.23263

Excited State 9: 1.000-A 0.6863 eV 1806.58 nm f=0.0000 <S**2>=0.000
435A -> 437A 0.57332
435A -> 438A -0.34727
436A -> 437A 0.16530
435B -> 437B 0.57332
435B -> 438B -0.34727
436B -> 437B 0.16530

Excited State 10: 3.000-A 0.7180 eV 1726.70 nm f=0.0000 <S**2>=2.000
432A -> 440A 0.13022
433A -> 437A 0.18354
433A -> 438A 0.24031
435A -> 439A -0.15641
435A -> 440A 0.13579
436A -> 439A -0.29948
436A -> 440A 0.46586
432B -> 440B -0.13022
433B -> 437B -0.18354
433B -> 438B -0.24031
435B -> 439B 0.15641

435B -> 440B -0.13579
436B -> 439B 0.29948
436B -> 440B -0.46586

Excited State 11: 1.000-A 0.7323 eV 1693.07 nm f=0.0029 <S**2>=0.000
434A -> 438A 0.14154
436A -> 438A 0.12182
436A -> 439A 0.52079
436A -> 440A -0.41579
434B -> 438B 0.14154
436B -> 438B 0.12182
436B -> 439B 0.52079
436B -> 440B -0.41579

Excited State 12: 3.000-A 0.7487 eV 1656.10 nm f=0.0000 <S**2>=2.000
433A -> 437A 0.13663
433A -> 438A 0.19950
434A -> 438A 0.11039
434A -> 439A -0.24169
434A -> 440A -0.11813
435A -> 437A -0.14505
435A -> 439A -0.29214
435A -> 440A 0.24997
436A -> 437A 0.19730
436A -> 439A 0.20087
436A -> 440A -0.23260
433B -> 437B -0.13663
433B -> 438B -0.19950
434B -> 438B -0.11039
434B -> 439B 0.24169
434B -> 440B 0.11813
435B -> 437B 0.14505
435B -> 439B 0.29214
435B -> 440B -0.24997
436B -> 437B -0.19730
436B -> 439B -0.20087

436B -> 440B 0.23260

Excited State 13: 3.000-A 0.7495 eV 1654.14 nm f=0.0000 <S**2>=2.000

430A -> 437A 0.10401
432A -> 437A -0.12647
433A -> 439A -0.10364
434A -> 438A 0.15751
434A -> 439A 0.27666
434A -> 440A 0.22313
435A -> 437A 0.10782
435A -> 438A -0.14979
435A -> 439A -0.28830
436A -> 437A -0.24168
436A -> 438A 0.24191
436A -> 440A -0.21447
430B -> 437B -0.10401
432B -> 437B 0.12647
433B -> 439B 0.10364
434B -> 438B -0.15751
434B -> 439B -0.27666
434B -> 440B -0.22313
435B -> 437B -0.10782
435B -> 438B 0.14979
435B -> 439B 0.28830
436B -> 437B 0.24168
436B -> 438B -0.24191
436B -> 440B 0.21447

Excited State 14: 1.000-A 0.7610 eV 1629.19 nm f=0.0027 <S**2>=0.000

433A -> 437A 0.12018
433A -> 438A -0.12844
435A -> 437A 0.13417
435A -> 438A 0.11072
435A -> 439A 0.53082
435A -> 440A 0.27955
436A -> 439A 0.18241

436A -> 440A 0.19567
433B -> 437B 0.12018
433B -> 438B -0.12844
435B -> 437B 0.13417
435B -> 438B 0.11072
435B -> 439B 0.53082
435B -> 440B 0.27955
436B -> 439B 0.18241
436B -> 440B 0.19567

Excited State 15: 3.000-A 0.7667 eV 1617.09 nm f=0.0000 <S**2>=2.000
433A -> 437A -0.14915
434A -> 437A -0.15198
435A -> 437A -0.14466
435A -> 439A -0.38646
435A -> 440A -0.49613
433B -> 437B 0.14915
434B -> 437B 0.15198
435B -> 437B 0.14466
435B -> 439B 0.38646
435B -> 440B 0.49613

Excited State 16: 1.000-A 0.7761 eV 1597.55 nm f=0.0192 <S**2>=0.000
432A -> 437A 0.10072
434A -> 439A -0.21445
435A -> 438A 0.32662
435A -> 439A -0.11494
436A -> 437A 0.47736
436A -> 438A -0.28455
432B -> 437B 0.10072
434B -> 439B -0.21445
435B -> 438B 0.32662
435B -> 439B -0.11494
436B -> 437B 0.47736
436B -> 438B -0.28455

Excited State 17: 3.000-A 0.7953 eV 1558.97 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 430A -> 438A | -0.12385 |
| 432A -> 437A | -0.11111 |
| 432A -> 438A | -0.15372 |
| 433A -> 439A | 0.29120 |
| 433A -> 440A | -0.31619 |
| 434A -> 439A | 0.11095 |
| 434A -> 440A | -0.10565 |
| 435A -> 437A | -0.20711 |
| 435A -> 438A | -0.38720 |
| 435A -> 439A | 0.15500 |
| 430B -> 438B | 0.12385 |
| 432B -> 437B | 0.11111 |
| 432B -> 438B | 0.15372 |
| 433B -> 439B | -0.29120 |
| 433B -> 440B | 0.31619 |
| 434B -> 439B | -0.11095 |
| 434B -> 440B | 0.10565 |
| 435B -> 437B | 0.20711 |
| 435B -> 438B | 0.38720 |
| 435B -> 439B | -0.15500 |

Excited State 18: 1.000-A 0.7985 eV 1552.72 nm f=0.0005 <S**2>=0.000

| | |
|---|---|
| 434A -> 437A | -0.36093 |
| 434A -> 438A | 0.13817 |
| 435A -> 439A | -0.18897 |
| 435A -> 440A | -0.20117 |
| 436A -> 439A | 0.29960 |
| 436A -> 440A | 0.42100 |
| 434B -> 437B | -0.36093 |
| 434B -> 438B | 0.13817 |
| 435B -> 439B | -0.18897 |
| 435B -> 440B | -0.20117 |
| 436B -> 439B | 0.29960 |
| 436B -> 440B | 0.42100 |

Excited State 19: 1.000-A 0.8411 eV 1473.99 nm f=0.1750 <S**2>=0.000

| | |
|---|---|
| 433A -> 437A | -0.10522 |
| 433A -> 438A | -0.10565 |
| 433A -> 439A | -0.17538 |
| 433A -> 440A | 0.13786 |
| 434A -> 440A | 0.13638 |
| 435A -> 437A | 0.32728 |
| 435A -> 438A | 0.42513 |
| 435A -> 440A | -0.11396 |
| 436A -> 437A | -0.16628 |
| 436A -> 438A | 0.26001 |
| 433B -> 437B | -0.10522 |
| 433B -> 438B | -0.10565 |
| 433B -> 439B | -0.17538 |
| 433B -> 440B | 0.13786 |
| 434B -> 440B | 0.13638 |
| 435B -> 437B | 0.32728 |
| 435B -> 438B | 0.42513 |
| 435B -> 440B | -0.11396 |
| 436B -> 437B | -0.16628 |
| 436B -> 438B | 0.26001 |

Excited State 20: 1.000-A 0.8430 eV 1470.73 nm f=0.0122 <S**2>=0.000

| | |
|---|---|
| 433A -> 437A | 0.26269 |
| 433A -> 438A | 0.22241 |
| 433A -> 439A | -0.12438 |
| 434A -> 438A | 0.12639 |
| 435A -> 439A | -0.28999 |
| 435A -> 440A | 0.47770 |
| 433B -> 437B | 0.26269 |
| 433B -> 438B | 0.22241 |
| 433B -> 439B | -0.12438 |
| 434B -> 438B | 0.12639 |
| 435B -> 439B | -0.28999 |
| 435B -> 440B | 0.47770 |

Excited State 21: 3.000-A 0.9587 eV 1293.23 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 433A -> 437A | -0.52990 |
| 433A -> 438A | 0.27812 |
| 434A -> 438A | 0.30446 |
| 435A -> 439A | 0.13010 |
| 435A -> 440A | 0.10337 |
| 433B -> 437B | 0.52990 |
| 433B -> 438B | -0.27812 |
| 434B -> 438B | -0.30446 |
| 435B -> 439B | -0.13010 |
| 435B -> 440B | -0.10337 |

Excited State 22: 1.000-A 0.9600 eV 1291.48 nm f=0.0001 <S**2>=0.000

| | |
|---|---|
| 433A -> 437A | 0.49344 |
| 433A -> 438A | -0.19681 |
| 434A -> 438A | -0.40458 |
| 435A -> 440A | -0.10063 |
| 436A -> 440A | -0.10944 |
| 433B -> 437B | 0.49344 |
| 433B -> 438B | -0.19681 |
| 434B -> 438B | -0.40458 |
| 435B -> 440B | -0.10063 |
| 436B -> 440B | -0.10944 |

Excited State 23: 3.000-A 0.9602 eV 1291.20 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 433A -> 438A | 0.30233 |
| 434A -> 437A | -0.37478 |
| 434A -> 438A | -0.45709 |
| 434A -> 439A | 0.11634 |
| 436A -> 440A | -0.10993 |
| 433B -> 438B | -0.30233 |
| 434B -> 437B | 0.37478 |
| 434B -> 438B | 0.45709 |
| 434B -> 439B | -0.11634 |
| 436B -> 440B | 0.10993 |

Excited State 24: 1.000-A 0.9636 eV 1286.67 nm f=0.0023 <S**2>=0.000

| | |
|---|---|
| 433A -> 437A | -0.20987 |
| 433A -> 438A | 0.37089 |
| 434A -> 437A | -0.36356 |
| 434A -> 438A | -0.36596 |
| 434A -> 439A | 0.10360 |
| 435A -> 440A | 0.13834 |
| 436A -> 440A | -0.10592 |
| 433B -> 437B | -0.20987 |
| 433B -> 438B | 0.37089 |
| 434B -> 437B | -0.36356 |
| 434B -> 438B | -0.36596 |
| 434B -> 439B | 0.10360 |
| 435B -> 440B | 0.13834 |
| 436B -> 440B | -0.10592 |

Excited State 25: 3.000-A 1.0293 eV 1204.54 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 433A -> 439A | -0.16046 |
| 433A -> 440A | 0.13701 |
| 434A -> 439A | 0.37902 |
| 434A -> 440A | -0.52765 |
| 433B -> 439B | 0.16046 |
| 433B -> 440B | -0.13701 |
| 434B -> 439B | -0.37902 |
| 434B -> 440B | 0.52765 |

Excited State 26: 1.000-A 1.0308 eV 1202.77 nm f=0.0018 <S**2>=0.000

| | |
|---|---|
| 433A -> 439A | 0.23289 |
| 434A -> 439A | -0.40684 |
| 434A -> 440A | 0.49224 |
| 433B -> 439B | 0.23289 |
| 434B -> 439B | -0.40684 |
| 434B -> 440B | 0.49224 |

Excited State 27: 3.000-A 1.0368 eV 1195.83 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 431A -> 439A | -0.11296 |

433A -> 437A -0.11807
433A -> 439A -0.47295
433A -> 440A -0.42019
434A -> 439A -0.17574
431B -> 439B 0.11296
433B -> 437B 0.11807
433B -> 439B 0.47295
433B -> 440B 0.42019
434B -> 439B 0.17574

Excited State 28: 1.000-A 1.0403 eV 1191.78 nm f=0.0016 <S**2>=0.000
433A -> 437A 0.12143
433A -> 439A 0.49107
433A -> 440A 0.39817
434A -> 439A 0.23246
435A -> 438A 0.11117
433B -> 437B 0.12143
433B -> 439B 0.49107
433B -> 440B 0.39817
434B -> 439B 0.23246
435B -> 438B 0.11117

Excited State 29: 3.000-A 1.0921 eV 1135.29 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.11929
429A -> 438A -0.11400
429A -> 439A -0.17110
429A -> 440A -0.14494
431A -> 437A 0.27574
431A -> 438A -0.24274
431A -> 439A -0.34621
431A -> 440A -0.25433
432A -> 437A -0.13588
433A -> 439A 0.11761
433A -> 440A 0.11148
429B -> 437B -0.11929
429B -> 438B 0.11400

429B -> 439B 0.17110
429B -> 440B 0.14494
431B -> 437B -0.27574
431B -> 438B 0.24274
431B -> 439B 0.34621
431B -> 440B 0.25433
432B -> 437B 0.13588
433B -> 439B -0.11761
433B -> 440B -0.11148

Excited State 30: 3.000-A 1.1128 eV 1114.14 nm f=0.0000 <S**2>=2.000
429A -> 437A -0.15910
429A -> 438A 0.13471
429A -> 439A -0.11031
429A -> 440A -0.13282
430A -> 437A 0.11100
430A -> 439A 0.11867
431A -> 437A -0.41362
431A -> 438A 0.11442
431A -> 439A -0.23501
431A -> 440A -0.11762
432A -> 437A -0.17771
432A -> 439A -0.17879
429B -> 437B 0.15910
429B -> 438B -0.13471
429B -> 439B 0.11031
429B -> 440B 0.13282
430B -> 437B -0.11100
430B -> 439B -0.11867
431B -> 437B 0.41362
431B -> 438B -0.11442
431B -> 439B 0.23501
431B -> 440B 0.11762
432B -> 437B 0.17771
432B -> 439B 0.17879

Excited State 31: 1.000-A 1.1206 eV 1106.42 nm f=0.0566 <S**2>=0.000

| | |
|---|---|
| 431A -> 438A | 0.10678 |
| 431A -> 439A | 0.22740 |
| 431A -> 440A | 0.13499 |
| 432A -> 437A | 0.20431 |
| 433A -> 440A | -0.22506 |
| 434A -> 439A | 0.36072 |
| 434A -> 440A | 0.33223 |
| 436A -> 437A | 0.15295 |
| 431B -> 438B | 0.10678 |
| 431B -> 439B | 0.22740 |
| 431B -> 440B | 0.13499 |
| 432B -> 437B | 0.20431 |
| 433B -> 440B | -0.22506 |
| 434B -> 439B | 0.36072 |
| 434B -> 440B | 0.33223 |
| 436B -> 437B | 0.15295 |

Excited State 32: 3.000-A 1.1354 eV 1092.02 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 429A -> 437A | 0.17707 |
| 429A -> 438A | 0.17165 |
| 429A -> 439A | 0.13340 |
| 429A -> 440A | -0.12730 |
| 431A -> 437A | -0.11663 |
| 431A -> 438A | -0.32800 |
| 431A -> 440A | 0.25941 |
| 432A -> 437A | -0.13626 |
| 432A -> 438A | -0.25827 |
| 432A -> 440A | 0.17526 |
| 433A -> 437A | -0.10300 |
| 433A -> 438A | -0.15620 |
| 433A -> 440A | 0.12793 |
| 429B -> 437B | -0.17707 |
| 429B -> 438B | -0.17165 |
| 429B -> 439B | -0.13340 |
| 429B -> 440B | 0.12730 |

431B -> 437B 0.11663
431B -> 438B 0.32800
431B -> 440B -0.25941
432B -> 437B 0.13626
432B -> 438B 0.25827
432B -> 440B -0.17526
433B -> 437B 0.10300
433B -> 438B 0.15620
433B -> 440B -0.12793

Excited State 33: 1.000-A 1.1500 eV 1078.17 nm f=0.0817 <S**2>=0.000
429A -> 438A -0.12130
431A -> 437A 0.27483
431A -> 440A -0.13352
432A -> 437A 0.14405
432A -> 438A 0.16618
433A -> 438A 0.30968
433A -> 439A 0.13140
433A -> 440A -0.29596
434A -> 437A 0.21540
435A -> 438A 0.12601
435A -> 440A -0.14036
436A -> 439A 0.11809
429B -> 438B -0.12130
431B -> 437B 0.27483
431B -> 440B -0.13352
432B -> 437B 0.14405
432B -> 438B 0.16618
433B -> 438B 0.30968
433B -> 439B 0.13140
433B -> 440B -0.29596
434B -> 437B 0.21540
435B -> 438B 0.12601
435B -> 440B -0.14036
436B -> 439B 0.11809

Excited State 34: 3.000-A 1.1567 eV 1071.86 nm f=0.0000 <S**2>=2.000

424A -> 437A 0.43572
424A -> 438A -0.34241
424A -> 439A -0.31814
424A -> 440A -0.24427
424B -> 437B -0.43572
424B -> 438B 0.34241
424B -> 439B 0.31814
424B -> 440B 0.24427

Excited State 35: 1.000-A 1.1719 eV 1058.00 nm f=0.0742 <S**2>=0.000

429A -> 437A 0.15540
430A -> 437A -0.13528
431A -> 437A 0.27534
431A -> 438A -0.21865
431A -> 440A 0.10859
432A -> 438A -0.14397
433A -> 437A -0.13034
433A -> 439A -0.15265
433A -> 440A 0.18895
434A -> 437A 0.25628
434A -> 438A -0.20811
434A -> 440A 0.17714
436A -> 439A 0.18769
436A -> 440A 0.17553
429B -> 437B 0.15540
430B -> 437B -0.13528
431B -> 437B 0.27534
431B -> 438B -0.21865
431B -> 440B 0.10859
432B -> 438B -0.14397
433B -> 437B -0.13034
433B -> 439B -0.15265
433B -> 440B 0.18895
434B -> 437B 0.25628
434B -> 438B -0.20811

434B -> 440B 0.17714
436B -> 439B 0.18769
436B -> 440B 0.17553

Excited State 36: 3.000-A 1.1806 eV 1050.19 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.10201
429A -> 440A 0.19483
430A -> 438A -0.26088
430A -> 439A -0.14183
430A -> 440A 0.19132
431A -> 437A 0.10162
431A -> 439A 0.23152
431A -> 440A -0.17606
432A -> 437A -0.28350
432A -> 438A -0.12203
432A -> 439A -0.12347
432A -> 440A 0.16638
433A -> 438A -0.14098
429B -> 439B 0.10201
429B -> 440B -0.19483
430B -> 438B 0.26088
430B -> 439B 0.14183
430B -> 440B -0.19132
431B -> 437B -0.10162
431B -> 439B -0.23152
431B -> 440B 0.17606
432B -> 437B 0.28350
432B -> 438B 0.12203
432B -> 439B 0.12347
432B -> 440B -0.16638
433B -> 438B 0.14098

Excited State 37: 3.000-A 1.1856 eV 1045.77 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.11364
430A -> 437A -0.28991
430A -> 438A 0.12493

430A -> 439A 0.13224
430A -> 440A 0.20198
431A -> 440A -0.13140
432A -> 437A 0.25342
432A -> 438A -0.26223
432A -> 439A -0.24936
434A -> 437A -0.12993
434A -> 439A 0.12824
434A -> 440A 0.13707
429B -> 439B 0.11364
430B -> 437B 0.28991
430B -> 438B -0.12493
430B -> 439B -0.13224
430B -> 440B -0.20198
431B -> 440B 0.13140
432B -> 437B -0.25342
432B -> 438B 0.26223
432B -> 439B 0.24936
434B -> 437B 0.12993
434B -> 439B -0.12824
434B -> 440B -0.13707

Excited State 38: 3.000-A 1.1887 eV 1043.02 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.12228
429A -> 438A 0.17346
429A -> 439A -0.16269
429A -> 440A 0.13165
430A -> 437A 0.10308
430A -> 438A 0.17188
430A -> 439A -0.13046
431A -> 437A -0.21774
431A -> 438A -0.29117
431A -> 439A 0.20600
431A -> 440A -0.24314
432A -> 437A 0.14243
432A -> 438A 0.14703

433A -> 440A -0.10216
429B -> 437B -0.12228
429B -> 438B -0.17346
429B -> 439B 0.16269
429B -> 440B -0.13165
430B -> 437B -0.10308
430B -> 438B -0.17188
430B -> 439B 0.13046
431B -> 437B 0.21774
431B -> 438B 0.29117
431B -> 439B -0.20600
431B -> 440B 0.24314
432B -> 437B -0.14243
432B -> 438B -0.14703
433B -> 440B 0.10216

Excited State 39: 3.000-A 1.1951 eV 1037.46 nm f=0.0000 <S**2>=2.000
423A -> 437A -0.42042
423A -> 438A 0.18571
423A -> 439A -0.34880
423A -> 440A -0.26528
423B -> 437B 0.42042
423B -> 438B -0.18571
423B -> 439B 0.34880
423B -> 440B 0.26528

Excited State 40: 3.000-A 1.2011 eV 1032.25 nm f=0.0000 <S**2>=2.000
421A -> 438A -0.11073
422A -> 437A -0.33083
422A -> 438A -0.48150
422A -> 439A -0.16033
422A -> 440A 0.29249
421B -> 438B 0.11073
422B -> 437B 0.33083
422B -> 438B 0.48150
422B -> 439B 0.16033

422B -> 440B -0.29249

Excited State 41: 3.000-A 1.2042 eV 1029.62 nm f=0.0000 <S**2>=2.000

423A -> 437A -0.13622
423A -> 439A -0.11396
429A -> 437A 0.10444
430A -> 437A 0.20268
430A -> 439A 0.22777
430A -> 440A 0.12200
431A -> 437A 0.18278
431A -> 438A -0.13683
431A -> 439A 0.17540
431A -> 440A 0.15598
432A -> 437A -0.16700
432A -> 438A 0.12021
432A -> 439A -0.25022
432A -> 440A -0.21871
434A -> 437A -0.13801
434A -> 439A -0.10834
434A -> 440A -0.11718
423B -> 437B 0.13622
423B -> 439B 0.11396
429B -> 437B -0.10444
430B -> 437B -0.20268
430B -> 439B -0.22777
430B -> 440B -0.12200
431B -> 437B -0.18278
431B -> 438B 0.13683
431B -> 439B -0.17540
431B -> 440B -0.15598
432B -> 437B 0.16700
432B -> 438B -0.12021
432B -> 439B 0.25022
432B -> 440B 0.21871
434B -> 437B 0.13801
434B -> 439B 0.10834

434B -> 440B 0.11718

Excited State 42: 3.000-A 1.2180 eV 1017.92 nm f=0.0000 <S**2>=2.000
425A -> 437A 0.23539
425A -> 438A 0.31824
425A -> 439A -0.38280
425A -> 440A 0.36292
425B -> 437B -0.23539
425B -> 438B -0.31824
425B -> 439B 0.38280
425B -> 440B -0.36292

Excited State 43: 3.000-A 1.2351 eV 1003.81 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.10626
430A -> 439A 0.19693
430A -> 440A -0.16585
431A -> 438A -0.14184
431A -> 439A 0.16256
431A -> 440A -0.16719
432A -> 437A -0.13419
432A -> 438A -0.20799
432A -> 439A 0.27862
432A -> 440A -0.30205
433A -> 438A 0.10414
433A -> 439A -0.11815
433A -> 440A 0.12624
429B -> 439B 0.10626
430B -> 439B -0.19693
430B -> 440B 0.16585
431B -> 438B 0.14184
431B -> 439B -0.16256
431B -> 440B 0.16719
432B -> 437B 0.13419
432B -> 438B 0.20799
432B -> 439B -0.27862
432B -> 440B 0.30205

433B -> 438B -0.10414
433B -> 439B 0.11815
433B -> 440B -0.12624

Excited State 44: 1.000-A 1.2432 eV 997.27 nm f=0.0037 <S**2>=0.000
429A -> 440A 0.15352
430A -> 438A -0.23872
431A -> 437A 0.10999
431A -> 438A 0.23782
431A -> 439A 0.35851
431A -> 440A 0.12929
432A -> 437A -0.35447
434A -> 439A -0.10258
429B -> 440B 0.15352
430B -> 438B -0.23872
431B -> 437B 0.10999
431B -> 438B 0.23782
431B -> 439B 0.35851
431B -> 440B 0.12929
432B -> 437B -0.35447
434B -> 439B -0.10258

Excited State 45: 1.000-A 1.2600 eV 984.01 nm f=0.0111 <S**2>=0.000
429A -> 437A 0.10635
429A -> 438A 0.15549
429A -> 439A 0.12779
430A -> 437A 0.28802
430A -> 438A 0.11608
430A -> 440A -0.10268
431A -> 437A -0.20039
431A -> 438A -0.27406
431A -> 439A 0.11997
431A -> 440A 0.25835
432A -> 438A 0.30034
429B -> 437B 0.10635
429B -> 438B 0.15549

429B -> 439B 0.12779
430B -> 437B 0.28802
430B -> 438B 0.11608
430B -> 440B -0.10268
431B -> 437B -0.20039
431B -> 438B -0.27406
431B -> 439B 0.11997
431B -> 440B 0.25835
432B -> 438B 0.30034

Excited State 46: 1.000-A 1.2715 eV 975.11 nm f=0.0128 <S**2>=0.000
430A -> 440A 0.11577
431A -> 437A 0.40373
431A -> 438A -0.12916
431A -> 439A 0.13027
431A -> 440A 0.13201
432A -> 439A -0.31257
433A -> 438A -0.17714
433A -> 439A 0.11303
434A -> 437A -0.23821
435A -> 440A 0.12741
430B -> 440B 0.11577
431B -> 437B 0.40373
431B -> 438B -0.12916
431B -> 439B 0.13027
431B -> 440B 0.13201
432B -> 439B -0.31257
433B -> 438B -0.17714
433B -> 439B 0.11303
434B -> 437B -0.23821
435B -> 440B 0.12741

Excited State 47: 1.000-A 1.2948 eV 957.53 nm f=0.0059 <S**2>=0.000
429A -> 439A 0.15201
429A -> 440A -0.14137
431A -> 437A 0.11011

431A -> 438A 0.36145
431A -> 439A -0.33736
431A -> 440A 0.31966
432A -> 438A 0.16316
432A -> 440A 0.15741
429B -> 439B 0.15201
429B -> 440B -0.14137
431B -> 437B 0.11011
431B -> 438B 0.36145
431B -> 439B -0.33736
431B -> 440B 0.31966
432B -> 438B 0.16316
432B -> 440B 0.15741

Excited State 48: 1.000-A 1.3257 eV 935.24 nm f=0.0357 <S**2>=0.000
430A -> 439A -0.21473
431A -> 437A -0.10123
431A -> 440A -0.22297
432A -> 440A 0.26893
433A -> 437A -0.20805
433A -> 438A -0.24356
433A -> 439A 0.16310
433A -> 440A -0.14296
434A -> 438A -0.20127
435A -> 439A -0.18207
435A -> 440A 0.17944
436A -> 440A 0.11831
430B -> 439B -0.21473
431B -> 437B -0.10123
431B -> 440B -0.22297
432B -> 440B 0.26893
433B -> 437B -0.20805
433B -> 438B -0.24356
433B -> 439B 0.16310
433B -> 440B -0.14296
434B -> 438B -0.20127

435B -> 439B -0.18207
435B -> 440B 0.17944
436B -> 440B 0.11831

Excited State 49: 1.000-A 1.3847 eV 895.37 nm f=0.0084 <S**2>=0.000
430A -> 437A 0.39430
430A -> 438A -0.24837
431A -> 439A 0.10189
432A -> 437A 0.42696
432A -> 438A -0.23170
433A -> 440A 0.10879
430B -> 437B 0.39430
430B -> 438B -0.24837
431B -> 439B 0.10189
432B -> 437B 0.42696
432B -> 438B -0.23170
433B -> 440B 0.10879

Excited State 50: 3.000-A 1.3853 eV 894.97 nm f=0.0000 <S**2>=2.000
430A -> 437A -0.50124
430A -> 438A 0.16964
432A -> 437A -0.27761
432A -> 438A 0.34832
430B -> 437B 0.50124
430B -> 438B -0.16964
432B -> 437B 0.27761
432B -> 438B -0.34832

Excited State 51: 1.000-A 1.3927 eV 890.27 nm f=0.0198 <S**2>=0.000
430A -> 437A -0.30581
430A -> 438A -0.33302
431A -> 439A 0.10965
432A -> 437A 0.25441
432A -> 438A 0.41093
433A -> 440A 0.12509
430B -> 437B -0.30581

430B -> 438B -0.33302
431B -> 439B 0.10965
432B -> 437B 0.25441
432B -> 438B 0.41093
433B -> 440B 0.12509

Excited State 52: 3.000-A 1.3967 eV 887.69 nm f=0.0000 <S**2>=2.000
430A -> 437A -0.14070
430A -> 438A -0.52358
431A -> 438A -0.16578
432A -> 437A 0.27898
432A -> 438A 0.24562
430B -> 437B 0.14070
430B -> 438B 0.52358
431B -> 438B 0.16578
432B -> 437B -0.27898
432B -> 438B -0.24562

Excited State 53: 1.000-A 1.4160 eV 875.58 nm f=0.0016 <S**2>=0.000
431A -> 437A 0.23339
432A -> 439A 0.54474
433A -> 438A -0.18681
434A -> 437A -0.12450
435A -> 440A 0.16259
436A -> 439A -0.12585
431B -> 437B 0.23339
432B -> 439B 0.54474
433B -> 438B -0.18681
434B -> 437B -0.12450
435B -> 440B 0.16259
436B -> 439B -0.12585

Excited State 54: 1.000-A 1.4359 eV 863.44 nm f=0.0482 <S**2>=0.000
429A -> 437A 0.19639
429A -> 438A 0.10182
430A -> 437A 0.10748

430A -> 438A 0.24590
430A -> 439A 0.13683
431A -> 438A 0.33191
431A -> 439A 0.14061
431A -> 440A -0.20461
432A -> 438A 0.16874
432A -> 439A -0.10903
432A -> 440A -0.23150
433A -> 440A 0.13025
435A -> 438A -0.13271
429B -> 437B 0.19639
429B -> 438B 0.10182
430B -> 437B 0.10748
430B -> 438B 0.24590
430B -> 439B 0.13683
431B -> 438B 0.33191
431B -> 439B 0.14061
431B -> 440B -0.20461
432B -> 438B 0.16874
432B -> 439B -0.10903
432B -> 440B -0.23150
433B -> 440B 0.13025
435B -> 438B -0.13271

Excited State 55: 1.000-A 1.4448 eV 858.13 nm f=0.0567 <S**2>=0.000
430A -> 438A 0.31641
430A -> 439A -0.20083
431A -> 439A 0.15269
432A -> 440A 0.41322
433A -> 439A -0.12035
433A -> 440A 0.15797
434A -> 439A -0.10762
435A -> 439A 0.10801
430B -> 438B 0.31641
430B -> 439B -0.20083
431B -> 439B 0.15269

432B -> 440B 0.41322
433B -> 439B -0.12035
433B -> 440B 0.15797
434B -> 439B -0.10762
435B -> 439B 0.10801

Excited State 56: 3.000-A 1.4483 eV 856.09 nm f=0.0000 <S**2>=2.000
428A -> 439A -0.10377
429A -> 437A -0.26307
429A -> 438A -0.20062
430A -> 439A -0.37463
430A -> 440A 0.14511
431A -> 438A -0.26172
432A -> 440A -0.32561
428B -> 439B 0.10377
429B -> 437B 0.26307
429B -> 438B 0.20062
430B -> 439B 0.37463
430B -> 440B -0.14511
431B -> 438B 0.26172
432B -> 440B 0.32561

Excited State 57: 3.000-A 1.4537 eV 852.86 nm f=0.0000 <S**2>=2.000
429A -> 438A 0.24717
430A -> 439A -0.24571
430A -> 440A -0.40300
431A -> 437A 0.16742
432A -> 439A -0.33928
432A -> 440A -0.16477
429B -> 438B -0.24717
430B -> 439B 0.24571
430B -> 440B 0.40300
431B -> 437B -0.16742
432B -> 439B 0.33928
432B -> 440B 0.16477

Excited State 58: 1.000-A 1.4586 eV 850.03 nm f=0.0902 <S**2>=0.000

| | |
|---|---|
| 429A -> 437A | 0.10080 |
| 430A -> 437A | -0.18631 |
| 430A -> 439A | 0.40578 |
| 431A -> 437A | -0.10633 |
| 431A -> 438A | 0.11898 |
| 431A -> 439A | 0.17955 |
| 431A -> 440A | 0.18751 |
| 432A -> 438A | -0.15116 |
| 432A -> 439A | 0.10979 |
| 432A -> 440A | 0.21943 |
| 434A -> 439A | -0.11043 |
| 434A -> 440A | -0.15281 |
| 436A -> 437A | -0.10816 |
| 429B -> 437B | 0.10080 |
| 430B -> 437B | -0.18631 |
| 430B -> 439B | 0.40578 |
| 431B -> 437B | -0.10633 |
| 431B -> 438B | 0.11898 |
| 431B -> 439B | 0.17955 |
| 431B -> 440B | 0.18751 |
| 432B -> 438B | -0.15116 |
| 432B -> 439B | 0.10979 |
| 432B -> 440B | 0.21943 |
| 434B -> 439B | -0.11043 |
| 434B -> 440B | -0.15281 |
| 436B -> 437B | -0.10816 |

Excited State 59: 1.000-A 1.4614 eV 848.39 nm f=0.0721 <S**2>=0.000

| | |
|---|---|
| 430A -> 437A | 0.20339 |
| 430A -> 438A | -0.13117 |
| 430A -> 439A | 0.38681 |
| 431A -> 439A | -0.13226 |
| 431A -> 440A | -0.21728 |
| 432A -> 437A | -0.11569 |
| 432A -> 438A | 0.11325 |

432A -> 440A 0.31626
434A -> 439A 0.15859
434A -> 440A 0.12457
436A -> 437A 0.12396
430B -> 437B 0.20339
430B -> 438B -0.13117
430B -> 439B 0.38681
431B -> 439B -0.13226
431B -> 440B -0.21728
432B -> 437B -0.11569
432B -> 438B 0.11325
432B -> 440B 0.31626
434B -> 439B 0.15859
434B -> 440B 0.12457
436B -> 437B 0.12396

Excited State 60: 3.000-A 1.4717 eV 842.46 nm f=0.0000 <S**2>=2.000
429A -> 437A -0.36862
429A -> 438A -0.23118
430A -> 439A 0.23555
430A -> 440A -0.28500
431A -> 438A -0.23674
432A -> 439A -0.13577
432A -> 440A 0.24749
429B -> 437B 0.36862
429B -> 438B 0.23118
430B -> 439B -0.23555
430B -> 440B 0.28500
431B -> 438B 0.23674
432B -> 439B 0.13577
432B -> 440B -0.24749

Excited State 61: 1.000-A 1.4811 eV 837.09 nm f=0.0100 <S**2>=0.000
429A -> 438A -0.23441
430A -> 440A 0.59235
431A -> 437A -0.10669

432A -> 439A 0.18007
429B -> 438B -0.23441
430B -> 440B 0.59235
431B -> 437B -0.10669
432B -> 439B 0.18007

Excited State 62: 3.000-A 1.4862 eV 834.24 nm f=0.0000 <S**2>=2.000
429A -> 437A 0.37035
429A -> 438A -0.42462
430A -> 440A -0.20215
431A -> 437A -0.26294
432A -> 439A -0.16992
429B -> 437B -0.37035
429B -> 438B 0.42462
430B -> 440B 0.20215
431B -> 437B 0.26294
432B -> 439B 0.16992

Excited State 63: 1.000-A 1.5134 eV 819.24 nm f=0.0118 <S**2>=0.000
429A -> 437A 0.56381
429A -> 438A 0.18077
429A -> 439A -0.11979
430A -> 438A -0.12608
430A -> 439A -0.17421
431A -> 438A 0.10369
429B -> 437B 0.56381
429B -> 438B 0.18077
429B -> 439B -0.11979
430B -> 438B -0.12608
430B -> 439B -0.17421
431B -> 438B 0.10369

Excited State 64: 3.000-A 1.5204 eV 815.47 nm f=0.0000 <S**2>=2.000
429A -> 439A -0.40596
429A -> 440A 0.34909
431A -> 439A -0.19441

431A -> 440A 0.35821
429B -> 439B 0.40596
429B -> 440B -0.34909
431B -> 439B 0.19441
431B -> 440B -0.35821

Excited State 65: 1.000-A 1.5370 eV 806.68 nm f=0.0145 <S**2>=0.000
424A -> 437A 0.14563
424A -> 438A -0.11281
424A -> 439A -0.10150
429A -> 437A -0.19622
429A -> 438A 0.53222
429A -> 440A 0.10410
430A -> 440A 0.24681
424B -> 437B 0.14563
424B -> 438B -0.11281
424B -> 439B -0.10150
429B -> 437B -0.19622
429B -> 438B 0.53222
429B -> 440B 0.10410
430B -> 440B 0.24681

Excited State 66: 3.000-A 1.5451 eV 802.44 nm f=0.0000 <S**2>=2.000
427A -> 437A -0.10852
429A -> 439A -0.38061
429A -> 440A -0.43651
431A -> 439A 0.29233
431A -> 440A 0.16295
427B -> 437B 0.10852
429B -> 439B 0.38061
429B -> 440B 0.43651
431B -> 439B -0.29233
431B -> 440B -0.16295

Excited State 67: 1.000-A 1.5527 eV 798.52 nm f=0.0070 <S**2>=0.000
424A -> 437A 0.40521

424A -> 438A -0.31499
424A -> 439A -0.28934
424A -> 440A -0.21999
429A -> 437A 0.11791
429A -> 438A -0.13130
429A -> 439A 0.14331
424B -> 437B 0.40521
424B -> 438B -0.31499
424B -> 439B -0.28934
424B -> 440B -0.21999
429B -> 437B 0.11791
429B -> 438B -0.13130
429B -> 439B 0.14331

Excited State 68: 1.000-A 1.5617 eV 793.93 nm f=0.0232 <S**2>=0.000
422A -> 438A 0.11505
429A -> 438A 0.13251
429A -> 439A 0.51524
429A -> 440A -0.28757
431A -> 440A -0.19525
422B -> 438B 0.11505
429B -> 438B 0.13251
429B -> 439B 0.51524
429B -> 440B -0.28757
431B -> 440B -0.19525

Excited State 69: 1.000-A 1.5805 eV 784.48 nm f=0.0008 <S**2>=0.000
423A -> 437A 0.39760
423A -> 438A -0.17429
423A -> 439A 0.32236
423A -> 440A 0.24296
429A -> 439A -0.10169
429A -> 440A -0.27027
423B -> 437B 0.39760
423B -> 438B -0.17429
423B -> 439B 0.32236

423B -> 440B 0.24296
429B -> 439B -0.10169
429B -> 440B -0.27027

Excited State 70: 1.000-A 1.5861 eV 781.71 nm f=0.0049 <S**2>=0.000
425A -> 437A -0.24802
425A -> 438A -0.32726
425A -> 439A 0.38773
425A -> 440A -0.36322
425B -> 437B -0.24802
425B -> 438B -0.32726
425B -> 439B 0.38773
425B -> 440B -0.36322

Excited State 71: 1.000-A 1.5915 eV 779.02 nm f=0.0199 <S**2>=0.000
422A -> 437A 0.28520
422A -> 438A 0.42681
422A -> 439A 0.13195
422A -> 440A -0.25427
423A -> 437A -0.14680
423A -> 439A -0.11399
429A -> 439A -0.20472
429A -> 440A -0.10227
422B -> 437B 0.28520
422B -> 438B 0.42681
422B -> 439B 0.13195
422B -> 440B -0.25427
423B -> 437B -0.14680
423B -> 439B -0.11399
429B -> 439B -0.20472
429B -> 440B -0.10227

Excited State 72: 1.000-A 1.5989 eV 775.42 nm f=0.0233 <S**2>=0.000
422A -> 437A 0.13937
422A -> 438A 0.17799
422A -> 440A -0.10452

423A -> 437A 0.14709
423A -> 439A 0.11754
429A -> 439A 0.25094
429A -> 440A 0.49084
430A -> 438A 0.10749
431A -> 439A -0.11161
422B -> 437B 0.13937
422B -> 438B 0.17799
422B -> 440B -0.10452
423B -> 437B 0.14709
423B -> 439B 0.11754
429B -> 439B 0.25094
429B -> 440B 0.49084
430B -> 438B 0.10749
431B -> 439B -0.11161

Excited State 73: 3.000-A 1.6418 eV 755.16 nm f=0.0000 <S**2>=2.000
427A -> 439A -0.17567
427A -> 440A 0.23719
428A -> 439A 0.38281
428A -> 440A -0.39666
429A -> 438A -0.11454
427B -> 439B 0.17567
427B -> 440B -0.23719
428B -> 439B -0.38281
428B -> 440B 0.39666
429B -> 438B 0.11454

Excited State 74: 3.000-A 1.6615 eV 746.24 nm f=0.0000 <S**2>=2.000
427A -> 437A 0.16807
427A -> 438A 0.19974
427A -> 439A -0.11352
427A -> 440A -0.14031
428A -> 437A -0.32772
428A -> 438A -0.46267
428A -> 439A -0.11346

429A -> 440A -0.13315
427B -> 437B -0.16807
427B -> 438B -0.19974
427B -> 439B 0.11352
427B -> 440B 0.14031
428B -> 437B 0.32772
428B -> 438B 0.46267
428B -> 439B 0.11346
429B -> 440B 0.13315

Excited State 75: 3.000-A 1.6627 eV 745.70 nm f=0.0000 <S**2>=2.000
427A -> 437A 0.10171
427A -> 438A -0.23048
427A -> 439A -0.36611
427A -> 440A -0.24185
428A -> 437A 0.22106
428A -> 439A -0.25874
428A -> 440A -0.27660
429A -> 438A -0.10685
427B -> 437B -0.10171
427B -> 438B 0.23048
427B -> 439B 0.36611
427B -> 440B 0.24185
428B -> 437B -0.22106
428B -> 439B 0.25874
428B -> 440B 0.27660
429B -> 438B 0.10685

Excited State 76: 3.000-A 1.6915 eV 732.98 nm f=0.0000 <S**2>=2.000
427A -> 437A -0.43610
427A -> 438A 0.17540
427A -> 439A -0.16978
427A -> 440A -0.11611
428A -> 437A -0.31352
428A -> 438A 0.22411
428A -> 439A -0.12754

428A -> 440A -0.12053
429A -> 439A 0.12325
429A -> 440A 0.13024
427B -> 437B 0.43610
427B -> 438B -0.17540
427B -> 439B 0.16978
427B -> 440B 0.11611
428B -> 437B 0.31352
428B -> 438B -0.22411
428B -> 439B 0.12754
428B -> 440B 0.12053
429B -> 439B -0.12325
429B -> 440B -0.13024

Excited State 77: 1.000-A 1.7015 eV 728.70 nm f=0.0006 <S**2>=0.000
427A -> 438A -0.22628
427A -> 440A 0.10997
428A -> 437A 0.43355
428A -> 438A 0.40693
428A -> 439A 0.13306
428A -> 440A -0.20496
427B -> 438B -0.22628
427B -> 440B 0.10997
428B -> 437B 0.43355
428B -> 438B 0.40693
428B -> 439B 0.13306
428B -> 440B -0.20496

Excited State 78: 1.000-A 1.7159 eV 722.57 nm f=0.0014 <S**2>=0.000
427A -> 437A 0.35457
427A -> 438A -0.20975
427A -> 439A -0.16979
427A -> 440A -0.18143
428A -> 437A 0.30867
428A -> 438A -0.30462
428A -> 439A -0.24965

427B -> 437B 0.35457
427B -> 438B -0.20975
427B -> 439B -0.16979
427B -> 440B -0.18143
428B -> 437B 0.30867
428B -> 438B -0.30462
428B -> 439B -0.24965

Excited State 79: 1.000-A 1.7390 eV 712.96 nm f=0.0010 <S**2>=0.000
427A -> 437A 0.27032
427A -> 439A 0.15760
427A -> 440A 0.27182
428A -> 438A -0.26485
428A -> 439A 0.47990
427B -> 437B 0.27032
427B -> 439B 0.15760
427B -> 440B 0.27182
428B -> 438B -0.26485
428B -> 439B 0.47990

Excited State 80: 1.000-A 1.7415 eV 711.95 nm f=0.0018 <S**2>=0.000
427A -> 439A 0.37757
428A -> 437A 0.21209
428A -> 438A 0.10040
428A -> 439A -0.10656
428A -> 440A 0.50725
427B -> 439B 0.37757
428B -> 437B 0.21209
428B -> 438B 0.10040
428B -> 439B -0.10656
428B -> 440B 0.50725

Excited State 81: 3.000-A 1.8244 eV 679.61 nm f=0.0000 <S**2>=2.000
420A -> 437A 0.18579
426A -> 439A -0.12029
427A -> 437A 0.23344

427A -> 438A -0.17456
428A -> 437A -0.38844
428A -> 438A 0.27449
420B -> 437B -0.18579
426B -> 439B 0.12029
427B -> 437B -0.23344
427B -> 438B 0.17456
428B -> 437B 0.38844
428B -> 438B -0.27449

Excited State 82: 3.000-A 1.8414 eV 673.31 nm f=0.0000 <S**2>=2.000
417A -> 438A 0.10930
419A -> 439A 0.12666
419A -> 440A -0.12666
420A -> 437A 0.10927
420A -> 438A 0.15580
427A -> 437A -0.16642
427A -> 438A -0.26218
428A -> 437A -0.13864
428A -> 438A -0.28058
428A -> 439A 0.13688
428A -> 440A -0.10215
417B -> 438B -0.10930
419B -> 439B -0.12666
419B -> 440B 0.12666
420B -> 437B -0.10927
420B -> 438B -0.15580
427B -> 437B 0.16642
427B -> 438B 0.26218
428B -> 437B 0.13864
428B -> 438B 0.28058
428B -> 439B -0.13688
428B -> 440B 0.10215

Excited State 83: 3.000-A 1.8537 eV 668.84 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.15270

411A -> 437A -0.11112
417A -> 439A -0.12365
418A -> 437A 0.15243
420A -> 439A 0.17275
420A -> 440A 0.14077
421A -> 437A -0.13516
426A -> 437A -0.21109
426A -> 438A 0.10635
427A -> 437A -0.10043
427A -> 438A 0.10347
427A -> 439A 0.10955
428A -> 437A 0.10462
428A -> 438A -0.10306
428A -> 439A -0.19892
428A -> 440A -0.18742
400B -> 437B -0.15270
411B -> 437B 0.11112
417B -> 439B 0.12365
418B -> 437B -0.15243
420B -> 439B -0.17275
420B -> 440B -0.14077
421B -> 437B 0.13516
426B -> 437B 0.21109
426B -> 438B -0.10635
427B -> 437B 0.10043
427B -> 438B -0.10347
427B -> 439B -0.10955
428B -> 437B -0.10462
428B -> 438B 0.10306
428B -> 439B 0.19892
428B -> 440B 0.18742

Excited State 84: 3.000-A 1.8583 eV 667.20 nm f=0.0000 <S**2>=2.000
399A -> 438A 0.14166
401A -> 438A 0.11849
410A -> 438A 0.12663

417A -> 437A -0.12222
417A -> 438A -0.18773
417A -> 440A 0.13569
419A -> 438A -0.11001
420A -> 438A -0.11130
420A -> 439A -0.11837
420A -> 440A 0.13404
426A -> 438A -0.14351
427A -> 440A -0.13331
428A -> 439A 0.13671
428A -> 440A -0.16014
399B -> 438B -0.14166
401B -> 438B -0.11849
410B -> 438B -0.12663
417B -> 437B 0.12222
417B -> 438B 0.18773
417B -> 440B -0.13569
419B -> 438B 0.11001
420B -> 438B 0.11130
420B -> 439B 0.11837
420B -> 440B -0.13404
426B -> 438B 0.14351
427B -> 440B 0.13331
428B -> 439B -0.13671
428B -> 440B 0.16014

Excited State 85: 1.000-A 1.8589 eV 666.97 nm f=0.0026 <S**2>=0.000
427A -> 437A 0.44668
427A -> 438A -0.21384
428A -> 437A -0.35893
428A -> 438A 0.33575
427B -> 437B 0.44668
427B -> 438B -0.21384
428B -> 437B -0.35893
428B -> 438B 0.33575

Excited State 86: 3.000-A 1.8894 eV 656.22 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 400A -> 439A | 0.13547 |
| 400A -> 440A | 0.10325 |
| 403A -> 437A | -0.11995 |
| 410A -> 437A | -0.10344 |
| 417A -> 437A | -0.17157 |
| 420A -> 437A | 0.13749 |
| 420A -> 438A | -0.11143 |
| 427A -> 437A | -0.26914 |
| 428A -> 437A | 0.17008 |
| 428A -> 438A | -0.14219 |
| 400B -> 439B | -0.13547 |
| 400B -> 440B | -0.10325 |
| 403B -> 437B | 0.11995 |
| 410B -> 437B | 0.10344 |
| 417B -> 437B | 0.17157 |
| 420B -> 437B | -0.13749 |
| 420B -> 438B | 0.11143 |
| 427B -> 437B | 0.26914 |
| 428B -> 437B | -0.17008 |
| 428B -> 438B | 0.14219 |

Excited State 87: 1.000-A 1.8975 eV 653.42 nm f=0.0085 <S**2>=0.000

| | |
|---|---|
| 427A -> 437A | 0.26638 |
| 427A -> 438A | 0.58102 |
| 428A -> 437A | 0.16420 |
| 428A -> 438A | 0.19086 |
| 427B -> 437B | 0.26638 |
| 427B -> 438B | 0.58102 |
| 428B -> 437B | 0.16420 |
| 428B -> 438B | 0.19086 |

Excited State 88: 3.000-A 1.9046 eV 650.96 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 417A -> 438A | -0.12932 |
| 427A -> 437A | -0.21440 |
| 427A -> 438A | -0.43902 |

428A -> 437A -0.11856
428A -> 438A -0.14011
417B -> 438B 0.12932
427B -> 437B 0.21440
427B -> 438B 0.43902
428B -> 437B 0.11856
428B -> 438B 0.14011

Excited State 89: 3.000-A 1.9191 eV 646.04 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.12334
411A -> 437A 0.11570
413A -> 437A -0.10056
427A -> 439A 0.28389
427A -> 440A 0.21596
428A -> 439A -0.32593
428A -> 440A -0.29075
400B -> 437B 0.12334
411B -> 437B -0.11570
413B -> 437B 0.10056
427B -> 439B -0.28389
427B -> 440B -0.21596
428B -> 439B 0.32593
428B -> 440B 0.29075

Excited State 90: 1.000-A 1.9270 eV 643.40 nm f=0.0009 <S**2>=0.000
427A -> 439A 0.37963
427A -> 440A 0.26555
428A -> 439A -0.35752
428A -> 440A -0.36311
427B -> 439B 0.37963
427B -> 440B 0.26555
428B -> 439B -0.35752
428B -> 440B -0.36311

Excited State 91: 3.000-A 1.9473 eV 636.71 nm f=0.0000 <S**2>=2.000
426A -> 437A -0.15542

426A -> 438A -0.17375
426A -> 439A 0.12669
427A -> 439A 0.26667
427A -> 440A -0.37333
428A -> 439A 0.14888
428A -> 440A -0.15683
426B -> 437B 0.15542
426B -> 438B 0.17375
426B -> 439B -0.12669
427B -> 439B -0.26667
427B -> 440B 0.37333
428B -> 439B -0.14888
428B -> 440B 0.15683

Excited State 92: 1.000-A 1.9615 eV 632.09 nm f=0.0022 <S**2>=0.000
427A -> 439A -0.34712
427A -> 440A 0.52708
428A -> 439A -0.18388
428A -> 440A 0.21030
427B -> 439B -0.34712
427B -> 440B 0.52708
428B -> 439B -0.18388
428B -> 440B 0.21030

Excited State 93: 3.000-A 1.9752 eV 627.71 nm f=0.0000 <S**2>=2.000
421A -> 438A 0.22204
426A -> 437A -0.44836
426A -> 438A -0.14394
427A -> 439A -0.23627
427A -> 440A 0.18093
428A -> 440A 0.12354
421B -> 438B -0.22204
426B -> 437B 0.44836
426B -> 438B 0.14394
427B -> 439B 0.23627
427B -> 440B -0.18093

428B -> 440B -0.12354

Excited State 94: 3.000-A 1.9826 eV 625.35 nm f=0.0000 <S**2>=2.000
407A -> 439A -0.11576
411A -> 437A -0.13465
421A -> 437A 0.25914
426A -> 437A 0.19580
426A -> 438A -0.42366
427A -> 440A 0.18056
407B -> 439B 0.11576
411B -> 437B 0.13465
421B -> 437B -0.25914
426B -> 437B -0.19580
426B -> 438B 0.42366
427B -> 440B -0.18056

Excited State 95: 3.000-A 1.9906 eV 622.84 nm f=0.0000 <S**2>=2.000
407A -> 438A -0.10271
411A -> 440A 0.13839
413A -> 439A -0.10296
421A -> 440A -0.21557
426A -> 437A -0.13448
426A -> 438A -0.17588
426A -> 439A -0.40508
426A -> 440A 0.16304
407B -> 438B 0.10271
411B -> 440B -0.13839
413B -> 439B 0.10296
421B -> 440B 0.21557
426B -> 437B 0.13448
426B -> 438B 0.17588
426B -> 439B 0.40508
426B -> 440B -0.16304

Excited State 96: 3.000-A 2.0021 eV 619.26 nm f=0.0000 <S**2>=2.000
407A -> 437A 0.11768

411A -> 439A 0.18391
413A -> 440A -0.12928
419A -> 440A 0.11930
421A -> 437A -0.13071
421A -> 438A -0.11043
421A -> 439A -0.13348
421A -> 440A -0.14420
426A -> 438A 0.13531
426A -> 439A -0.31882
426A -> 440A -0.20065
407B -> 437B -0.11768
411B -> 439B -0.18391
413B -> 440B 0.12928
419B -> 440B -0.11930
421B -> 437B 0.13071
421B -> 438B 0.11043
421B -> 439B 0.13348
421B -> 440B 0.14420
426B -> 438B -0.13531
426B -> 439B 0.31882
426B -> 440B 0.20065

Excited State 97: 3.000-A 2.0073 eV 617.68 nm f=0.0000 <S**2>=2.000
411A -> 440A 0.10212
413A -> 439A -0.11904
419A -> 439A 0.12052
421A -> 439A -0.28314
426A -> 440A -0.42366
411B -> 440B -0.10212
413B -> 439B 0.11904
419B -> 439B -0.12052
421B -> 439B 0.28314
426B -> 440B 0.42366

Excited State 98: 1.000-A 2.0218 eV 613.24 nm f=0.0095 <S**2>=0.000
421A -> 437A 0.14546

421A -> 438A -0.22339
425A -> 437A 0.10375
426A -> 437A 0.61978
421B -> 437B 0.14546
421B -> 438B -0.22339
425B -> 437B 0.10375
426B -> 437B 0.61978

Excited State 99: 1.000-A 2.0483 eV 605.32 nm f=0.0008 <S**2>=0.000
421A -> 437A -0.30424
426A -> 438A 0.58313
421B -> 437B -0.30424
426B -> 438B 0.58313

Excited State 100: 3.000-A 2.0535 eV 603.76 nm f=0.0000 <S**2>=2.000
402A -> 438A 0.12075
404A -> 437A -0.12400
404A -> 438A -0.13240
405A -> 437A -0.10166
405A -> 438A -0.18655
405A -> 440A 0.11460
406A -> 438A 0.11613
409A -> 438A 0.14782
410A -> 438A -0.10658
412A -> 438A 0.10387
415A -> 437A -0.18138
415A -> 438A -0.19756
415A -> 439A -0.10155
415A -> 440A 0.10851
421A -> 437A -0.10311
421A -> 438A -0.10979
402B -> 438B -0.12075
404B -> 437B 0.12400
404B -> 438B 0.13240
405B -> 437B 0.10166
405B -> 438B 0.18655

405B -> 440B -0.11460
406B -> 438B -0.11613
409B -> 438B -0.14782
410B -> 438B 0.10658
412B -> 438B -0.10387
415B -> 437B 0.18138
415B -> 438B 0.19756
415B -> 439B 0.10155
415B -> 440B -0.10851
421B -> 437B 0.10311
421B -> 438B 0.10979

Excited State 101: 3.000-A 2.0672 eV 599.78 nm f=0.0000 <S**2>=2.000
403A -> 437A -0.15517
403A -> 439A -0.15032
403A -> 440A -0.10925
404A -> 437A 0.15012
404A -> 438A -0.10007
404A -> 439A 0.13000
404A -> 440A 0.12115
405A -> 437A -0.17427
405A -> 439A -0.13084
406A -> 437A 0.15045
406A -> 439A 0.11994
415A -> 437A 0.17238
415A -> 438A -0.12001
415A -> 439A 0.15214
415A -> 440A 0.14469
403B -> 437B 0.15517
403B -> 439B 0.15032
403B -> 440B 0.10925
404B -> 437B -0.15012
404B -> 438B 0.10007
404B -> 439B -0.13000
404B -> 440B -0.12115
405B -> 437B 0.17427

405B -> 439B 0.13084
406B -> 437B -0.15045
406B -> 439B -0.11994
415B -> 437B -0.17238
415B -> 438B 0.12001
415B -> 439B -0.15214
415B -> 440B -0.14469

Excited State 102: 3.000-A 2.0756 eV 597.35 nm f=0.0000 <S**2>=2.000
403A -> 437A -0.13569
403A -> 438A 0.10509
407A -> 437A 0.11145
409A -> 437A 0.15448
409A -> 438A -0.11848
409A -> 439A -0.10510
413A -> 437A 0.12619
413A -> 439A -0.10315
416A -> 437A -0.14379
416A -> 438A 0.10896
416A -> 439A 0.10455
420A -> 437A 0.12488
425A -> 437A -0.18614
425A -> 438A 0.14955
425A -> 439A 0.10378
403B -> 437B 0.13569
403B -> 438B -0.10509
407B -> 437B -0.11145
409B -> 437B -0.15448
409B -> 438B 0.11848
409B -> 439B 0.10510
413B -> 437B -0.12619
413B -> 439B 0.10315
416B -> 437B 0.14379
416B -> 438B -0.10896
416B -> 439B -0.10455
420B -> 437B -0.12488

425B -> 437B 0.18614
425B -> 438B -0.14955
425B -> 439B -0.10378

Excited State 103: 1.000-A 2.0835 eV 595.09 nm f=0.0228 <S**2>=0.000
421A -> 439A 0.17076
421A -> 440A 0.21721
425A -> 439A 0.13393
426A -> 439A 0.54919
426A -> 440A 0.12637
421B -> 439B 0.17076
421B -> 440B 0.21721
425B -> 439B 0.13393
426B -> 439B 0.54919
426B -> 440B 0.12637

Excited State 104: 1.000-A 2.1002 eV 590.35 nm f=0.0225 <S**2>=0.000
421A -> 439A 0.28212
421A -> 440A -0.13511
425A -> 437A -0.17967
425A -> 438A 0.16445
425A -> 440A 0.13382
426A -> 439A -0.26410
426A -> 440A 0.45021
421B -> 439B 0.28212
421B -> 440B -0.13511
425B -> 437B -0.17967
425B -> 438B 0.16445
425B -> 440B 0.13382
426B -> 439B -0.26410
426B -> 440B 0.45021

Excited State 105: 3.000-A 2.1036 eV 589.39 nm f=0.0000 <S**2>=2.000
425A -> 437A -0.41774
425A -> 438A 0.33344
425A -> 439A 0.20354

425A -> 440A 0.19289
426A -> 437A 0.10586
425B -> 437B 0.41774
425B -> 438B -0.33344
425B -> 439B -0.20354
425B -> 440B -0.19289
426B -> 437B -0.10586

Excited State 106: 1.000-A 2.1070 eV 588.44 nm f=0.0122 <S**2>=0.000
421A -> 439A 0.18045
425A -> 437A 0.42565
425A -> 438A -0.33104
425A -> 439A -0.18564
425A -> 440A -0.16994
426A -> 438A 0.11700
426A -> 440A 0.27747
421B -> 439B 0.18045
425B -> 437B 0.42565
425B -> 438B -0.33104
425B -> 439B -0.18564
425B -> 440B -0.16994
426B -> 438B 0.11700
426B -> 440B 0.27747

Excited State 107: 3.000-A 2.1331 eV 581.24 nm f=0.0000 <S**2>=2.000
403A -> 437A 0.11405
416A -> 437A 0.14313
416A -> 438A -0.10992
418A -> 437A -0.17405
420A -> 437A 0.19570
420A -> 438A -0.16467
420A -> 439A -0.16455
421A -> 437A -0.33150
426A -> 438A -0.14340
403B -> 437B -0.11405
416B -> 437B -0.14313

416B -> 438B 0.10992
418B -> 437B 0.17405
420B -> 437B -0.19570
420B -> 438B 0.16467
420B -> 439B 0.16455
421B -> 437B 0.33150
426B -> 438B 0.14340

Excited State 108: 3.000-A 2.1397 eV 579.46 nm f=0.0000 <S**2>=2.000
418A -> 437A -0.10243
420A -> 437A -0.32405
421A -> 437A -0.26504
421A -> 438A -0.21412
426A -> 438A -0.16682
427A -> 438A -0.10089
418B -> 437B 0.10243
420B -> 437B 0.32405
421B -> 437B 0.26504
421B -> 438B 0.21412
426B -> 438B 0.16682
427B -> 438B 0.10089

Excited State 109: 3.000-A 2.1524 eV 576.03 nm f=0.0000 <S**2>=2.000
418A -> 437A 0.12068
418A -> 438A -0.10504
420A -> 437A 0.14254
420A -> 438A -0.24521
421A -> 437A 0.16210
421A -> 438A -0.35187
421A -> 439A 0.10107
421A -> 440A 0.12048
426A -> 437A -0.17235
418B -> 437B -0.12068
418B -> 438B 0.10504
420B -> 437B -0.14254
420B -> 438B 0.24521

421B -> 437B -0.16210
421B -> 438B 0.35187
421B -> 439B -0.10107
421B -> 440B -0.12048
426B -> 437B 0.17235

Excited State 110: 1.000-A 2.1535 eV 575.73 nm f=0.0049 <S**2>=0.000
418A -> 437A 0.19364
420A -> 437A -0.27234
420A -> 438A 0.15288
421A -> 437A 0.43101
421A -> 438A -0.13307
422A -> 437A -0.11980
423A -> 437A 0.12301
426A -> 437A -0.13714
426A -> 438A 0.22675
418B -> 437B 0.19364
420B -> 437B -0.27234
420B -> 438B 0.15288
421B -> 437B 0.43101
421B -> 438B -0.13307
422B -> 437B -0.11980
423B -> 437B 0.12301
426B -> 437B -0.13714
426B -> 438B 0.22675

Excited State 111: 1.000-A 2.1602 eV 573.95 nm f=0.0534 <S**2>=0.000
417A -> 438A 0.14606
419A -> 437A 0.12865
420A -> 437A 0.48698
421A -> 437A 0.30933
421A -> 438A 0.14283
426A -> 438A 0.17400
417B -> 438B 0.14606
419B -> 437B 0.12865
420B -> 437B 0.48698

421B -> 437B 0.30933
421B -> 438B 0.14283
426B -> 438B 0.17400

Excited State 112: 3.000-A 2.1620 eV 573.46 nm f=0.0000 <S**2>=2.000
414A -> 439A -0.10338
414A -> 440A 0.10682
419A -> 437A 0.12590
419A -> 438A 0.16348
419A -> 439A -0.19873
419A -> 440A 0.18080
420A -> 437A -0.16044
420A -> 438A -0.28479
420A -> 440A -0.10425
421A -> 437A 0.10023
421A -> 438A 0.19565
421A -> 439A -0.15229
421A -> 440A 0.13876
414B -> 439B 0.10338
414B -> 440B -0.10682
419B -> 437B -0.12590
419B -> 438B -0.16348
419B -> 439B 0.19873
419B -> 440B -0.18080
420B -> 437B 0.16044
420B -> 438B 0.28479
420B -> 440B 0.10425
421B -> 437B -0.10023
421B -> 438B -0.19565
421B -> 439B 0.15229
421B -> 440B -0.13876

Excited State 113: 1.000-A 2.1740 eV 570.30 nm f=0.0007 <S**2>=0.000
417A -> 437A 0.13424
419A -> 438A 0.14049
420A -> 437A -0.10241

420A -> 438A 0.25598
421A -> 438A 0.50782
422A -> 438A -0.10257
426A -> 437A 0.17903
417B -> 437B 0.13424
419B -> 438B 0.14049
420B -> 437B -0.10241
420B -> 438B 0.25598
421B -> 438B 0.50782
422B -> 438B -0.10257
426B -> 437B 0.17903

Excited State 114: 3.000-A 2.1860 eV 567.18 nm f=0.0000 <S**2>=2.000
400A -> 437A 0.12307
408A -> 437A 0.12459
418A -> 439A -0.11945
420A -> 439A -0.36429
420A -> 440A -0.11997
421A -> 437A 0.20184
421A -> 439A -0.14843
421A -> 440A -0.13293
426A -> 437A -0.13528
426A -> 438A 0.20222
400B -> 437B -0.12307
408B -> 437B -0.12459
418B -> 439B 0.11945
420B -> 439B 0.36429
420B -> 440B 0.11997
421B -> 437B -0.20184
421B -> 439B 0.14843
421B -> 440B 0.13293
426B -> 437B 0.13528
426B -> 438B -0.20222

Excited State 115: 1.000-A 2.1866 eV 567.02 nm f=0.0153 <S**2>=0.000
417A -> 437A 0.14190

417A -> 438A 0.12358
419A -> 439A 0.10306
420A -> 437A 0.23077
420A -> 438A 0.48633
421A -> 438A -0.18410
423A -> 438A -0.10222
426A -> 438A -0.13096
417B -> 437B 0.14190
417B -> 438B 0.12358
419B -> 439B 0.10306
420B -> 437B 0.23077
420B -> 438B 0.48633
421B -> 438B -0.18410
423B -> 438B -0.10222
426B -> 438B -0.13096

Excited State 116: 3.000-A 2.1972 eV 564.29 nm f=0.0000 <S**2>=2.000
399A -> 438A 0.10322
418A -> 439A -0.10046
419A -> 439A -0.15760
420A -> 437A 0.18770
420A -> 438A 0.11740
420A -> 439A 0.12744
420A -> 440A -0.21262
421A -> 438A -0.24295
421A -> 439A -0.18650
426A -> 437A -0.13250
426A -> 438A -0.15013
426A -> 439A 0.12193
426A -> 440A 0.13455
399B -> 438B -0.10322
418B -> 439B 0.10046
419B -> 439B 0.15760
420B -> 437B -0.18770
420B -> 438B -0.11740
420B -> 439B -0.12744

420B -> 440B 0.21262
421B -> 438B 0.24295
421B -> 439B 0.18650
426B -> 437B 0.13250
426B -> 438B 0.15013
426B -> 439B -0.12193
426B -> 440B -0.13455

Excited State 117: 3.000-A 2.2110 eV 560.76 nm f=0.0000 <S**2>=2.000
418A -> 439A -0.10437
420A -> 437A 0.19655
420A -> 440A 0.27281
421A -> 438A 0.10555
421A -> 439A -0.34275
426A -> 437A 0.12838
426A -> 439A 0.11343
426A -> 440A 0.25027
418B -> 439B 0.10437
420B -> 437B -0.19655
420B -> 440B -0.27281
421B -> 438B -0.10555
421B -> 439B 0.34275
426B -> 437B -0.12838
426B -> 439B -0.11343
426B -> 440B -0.25027

Excited State 118: 1.000-A 2.2167 eV 559.32 nm f=0.0048 <S**2>=0.000
418A -> 439A 0.19935
419A -> 439A 0.16831
421A -> 439A 0.46862
422A -> 439A -0.11602
423A -> 439A 0.10882
426A -> 439A -0.10708
426A -> 440A -0.36638
418B -> 439B 0.19935
419B -> 439B 0.16831

421B -> 439B 0.46862
422B -> 439B -0.11602
423B -> 439B 0.10882
426B -> 439B -0.10708
426B -> 440B -0.36638

Excited State 119: 3.000-A 2.2177 eV 559.06 nm f=0.0000 <S**2>=2.000
418A -> 440A -0.10092
419A -> 440A -0.13156
420A -> 438A -0.26322
420A -> 439A 0.20538
420A -> 440A -0.11573
421A -> 440A -0.40144
426A -> 439A 0.20926
418B -> 440B 0.10092
419B -> 440B 0.13156
420B -> 438B 0.26322
420B -> 439B -0.20538
420B -> 440B 0.11573
421B -> 440B 0.40144
426B -> 439B -0.20926

Excited State 120: 1.000-A 2.2237 eV 557.56 nm f=0.0066 <S**2>=0.000
417A -> 439A -0.14012
418A -> 437A 0.30917
418A -> 438A -0.10427
420A -> 437A 0.10303
420A -> 438A -0.13001
420A -> 439A 0.44729
420A -> 440A 0.20899
417B -> 439B -0.14012
418B -> 437B 0.30917
418B -> 438B -0.10427
420B -> 437B 0.10303
420B -> 438B -0.13001
420B -> 439B 0.44729

420B -> 440B 0.20899

Excited State 121: 1.000-A 2.2413 eV 553.18 nm f=0.0006 <S**2>=0.000

416A -> 437A -0.14230
416A -> 438A 0.13194
418A -> 440A 0.13847
419A -> 437A 0.14409
419A -> 439A -0.14655
419A -> 440A 0.13626
420A -> 438A 0.10593
421A -> 440A 0.46528
422A -> 440A -0.11400
423A -> 440A 0.11642
424A -> 440A 0.12166
426A -> 439A -0.19840
416B -> 437B -0.14230
416B -> 438B 0.13194
418B -> 440B 0.13847
419B -> 437B 0.14409
419B -> 439B -0.14655
419B -> 440B 0.13626
420B -> 438B 0.10593
421B -> 440B 0.46528
422B -> 440B -0.11400
423B -> 440B 0.11642
424B -> 440B 0.12166
426B -> 439B -0.19840

Excited State 122: 1.000-A 2.2419 eV 553.02 nm f=0.0028 <S**2>=0.000

416A -> 437A 0.15333
416A -> 438A -0.15745
416A -> 440A -0.12039
417A -> 438A -0.12065
419A -> 437A -0.24514
419A -> 439A 0.17262
420A -> 439A -0.26679

420A -> 440A 0.25309
421A -> 440A 0.27830
426A -> 439A -0.13492
416B -> 437B 0.15333
416B -> 438B -0.15745
416B -> 440B -0.12039
417B -> 438B -0.12065
419B -> 437B -0.24514
419B -> 439B 0.17262
420B -> 439B -0.26679
420B -> 440B 0.25309
421B -> 440B 0.27830
426B -> 439B -0.13492

Excited State 123: 3.000-A 2.2427 eV 552.83 nm f=0.0000 <S**2>=2.000
399A -> 439A -0.11249
399A -> 440A 0.10989
404A -> 440A 0.10638
419A -> 437A 0.10375
419A -> 438A 0.11905
420A -> 439A -0.10759
420A -> 440A 0.11954
421A -> 439A 0.13949
421A -> 440A -0.21289
426A -> 439A 0.17331
426A -> 440A -0.18918
399B -> 439B 0.11249
399B -> 440B -0.10989
404B -> 440B -0.10638
419B -> 437B -0.10375
419B -> 438B -0.11905
420B -> 439B 0.10759
420B -> 440B -0.11954
421B -> 439B -0.13949
421B -> 440B 0.21289
426B -> 439B -0.17331

426B -> 440B 0.18918

Excited State 124: 3.000-A 2.2485 eV 551.41 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.17040
395A -> 438A -0.13400
395A -> 439A -0.12455
403A -> 437A 0.14042
403A -> 438A -0.10952
416A -> 437A -0.28138
416A -> 438A 0.20619
416A -> 439A 0.19656
416A -> 440A 0.13539
417A -> 437A -0.13578
419A -> 437A 0.13176
419A -> 438A -0.10728
395B -> 437B -0.17040
395B -> 438B 0.13400
395B -> 439B 0.12455
403B -> 437B -0.14042
403B -> 438B 0.10952
416B -> 437B 0.28138
416B -> 438B -0.20619
416B -> 439B -0.19656
416B -> 440B -0.13539
417B -> 437B 0.13578
419B -> 437B -0.13176
419B -> 438B 0.10728

Excited State 125: 1.000-A 2.2502 eV 551.00 nm f=0.0078 <S**2>=0.000
416A -> 437A 0.30072
416A -> 438A -0.18712
416A -> 439A -0.21747
416A -> 440A -0.12495
417A -> 437A 0.13939
419A -> 438A 0.18090
419A -> 440A 0.12876

420A -> 440A -0.26193
424A -> 437A 0.15171
424A -> 438A 0.21416
424A -> 439A -0.13839
424A -> 440A 0.15752
416B -> 437B 0.30072
416B -> 438B -0.18712
416B -> 439B -0.21747
416B -> 440B -0.12495
417B -> 437B 0.13939
419B -> 438B 0.18090
419B -> 440B 0.12876
420B -> 440B -0.26193
424B -> 437B 0.15171
424B -> 438B 0.21416
424B -> 439B -0.13839
424B -> 440B 0.15752

Excited State 126: 1.000-A 2.2533 eV 550.24 nm f=0.0041 <S**2>=0.000
416A -> 437A -0.12989
416A -> 439A 0.10371
419A -> 438A -0.12231
419A -> 440A -0.11791
420A -> 440A 0.17593
421A -> 440A -0.13911
424A -> 437A 0.26358
424A -> 438A 0.39559
424A -> 439A -0.24628
424A -> 440A 0.23865
416B -> 437B -0.12989
416B -> 439B 0.10371
419B -> 438B -0.12231
419B -> 440B -0.11791
420B -> 440B 0.17593
421B -> 440B -0.13911
424B -> 437B 0.26358

424B -> 438B 0.39559
424B -> 439B -0.24628
424B -> 440B 0.23865

Excited State 127: 3.000-A 2.2537 eV 550.13 nm f=0.0000 <S**2>=2.000
424A -> 437A 0.30951
424A -> 438A 0.44714
424A -> 439A -0.28442
424A -> 440A 0.29266
424B -> 437B -0.30951
424B -> 438B -0.44714
424B -> 439B 0.28442
424B -> 440B -0.29266

Excited State 128: 3.000-A 2.2665 eV 547.02 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.14386
400A -> 439A -0.11918
402A -> 437A 0.13892
402A -> 439A 0.11402
404A -> 439A 0.11528
412A -> 437A -0.14066
417A -> 437A -0.19404
417A -> 439A -0.11392
418A -> 437A 0.15149
418A -> 439A 0.10582
420A -> 437A -0.10851
420A -> 438A 0.11572
420A -> 439A -0.12357
420A -> 440A -0.16858
400B -> 437B 0.14386
400B -> 439B 0.11918
402B -> 437B -0.13892
402B -> 439B -0.11402
404B -> 439B -0.11528
412B -> 437B 0.14066
417B -> 437B 0.19404

417B -> 439B 0.11392
418B -> 437B -0.15149
418B -> 439B -0.10582
420B -> 437B 0.10851
420B -> 438B -0.11572
420B -> 439B 0.12357
420B -> 440B 0.16858

Excited State 129: 3.000-A 2.2736 eV 545.33 nm f=0.0000 <S**2>=2.000
401A -> 437A -0.12556
401A -> 438A -0.19154
401A -> 440A 0.12619
404A -> 437A -0.11236
405A -> 438A -0.12402
412A -> 438A -0.15213
413A -> 438A 0.13767
417A -> 438A -0.18044
418A -> 437A -0.12297
423A -> 437A -0.13688
423A -> 438A -0.23528
401B -> 437B 0.12556
401B -> 438B 0.19154
401B -> 440B -0.12619
404B -> 437B 0.11236
405B -> 438B 0.12402
412B -> 438B 0.15213
413B -> 438B -0.13767
417B -> 438B 0.18044
418B -> 437B 0.12297
423B -> 437B 0.13688
423B -> 438B 0.23528

Excited State 130: 1.000-A 2.2842 eV 542.78 nm f=0.0026 <S**2>=0.000
412A -> 438A -0.13026
415A -> 437A 0.16999
415A -> 438A 0.15176

418A -> 437A -0.13210
418A -> 438A -0.15940
423A -> 437A 0.26974
423A -> 438A 0.44735
423A -> 440A -0.16211
412B -> 438B -0.13026
415B -> 437B 0.16999
415B -> 438B 0.15176
418B -> 437B -0.13210
418B -> 438B -0.15940
423B -> 437B 0.26974
423B -> 438B 0.44735
423B -> 440B -0.16211

Excited State 131: 3.000-A 2.2870 eV 542.12 nm f=0.0000 <S**2>=2.000
418A -> 437A 0.15827
420A -> 438A -0.11238
421A -> 438A 0.11724
423A -> 437A -0.29959
423A -> 438A -0.46997
423A -> 440A 0.17999
418B -> 437B -0.15827
420B -> 438B 0.11238
421B -> 438B -0.11724
423B -> 437B 0.29959
423B -> 438B 0.46997
423B -> 440B -0.17999

Excited State 132: 1.000-A 2.2873 eV 542.06 nm f=0.0226 <S**2>=0.000
414A -> 437A -0.10540
414A -> 438A -0.14961
414A -> 439A 0.18720
414A -> 440A -0.17961
415A -> 437A -0.12820
417A -> 437A 0.11211
418A -> 437A 0.14882

418A -> 438A 0.21519
418A -> 439A -0.15154
418A -> 440A 0.10852
419A -> 438A -0.11777
419A -> 439A 0.12937
419A -> 440A -0.11019
420A -> 439A 0.10286
420A -> 440A -0.16521
423A -> 438A 0.17017
414B -> 437B -0.10540
414B -> 438B -0.14961
414B -> 439B 0.18720
414B -> 440B -0.17961
415B -> 437B -0.12820
417B -> 437B 0.11211
418B -> 437B 0.14882
418B -> 438B 0.21519
418B -> 439B -0.15154
418B -> 440B 0.10852
419B -> 438B -0.11777
419B -> 439B 0.12937
419B -> 440B -0.11019
420B -> 439B 0.10286
420B -> 440B -0.16521
423B -> 438B 0.17017

Excited State 133: 1.000-A 2.2885 eV 541.77 nm f=0.0055 <S**2>=0.000
412A -> 438A 0.18713
412A -> 440A -0.12553
415A -> 437A -0.25770
415A -> 438A -0.15554
415A -> 439A -0.16429
417A -> 438A -0.15161
418A -> 440A -0.11171
419A -> 437A 0.13677
420A -> 438A 0.10400

423A -> 437A 0.15589
423A -> 438A 0.27012
423A -> 440A -0.11342
425A -> 437A -0.13383
425A -> 438A -0.10798
425A -> 439A -0.13447
412B -> 438B 0.18713
412B -> 440B -0.12553
415B -> 437B -0.25770
415B -> 438B -0.15554
415B -> 439B -0.16429
417B -> 438B -0.15161
418B -> 440B -0.11171
419B -> 437B 0.13677
420B -> 438B 0.10400
423B -> 437B 0.15589
423B -> 438B 0.27012
423B -> 440B -0.11342
425B -> 437B -0.13383
425B -> 438B -0.10798
425B -> 439B -0.13447

Excited State 134: 3.000-A 2.2911 eV 541.15 nm f=0.0000 <S**2>=2.000
425A -> 437A -0.42127
425A -> 438A -0.31394
425A -> 439A -0.41553
425A -> 440A 0.11128
425B -> 437B 0.42127
425B -> 438B 0.31394
425B -> 439B 0.41553
425B -> 440B -0.11128

Excited State 135: 1.000-A 2.2927 eV 540.79 nm f=0.0006 <S**2>=0.000
415A -> 438A -0.11039
417A -> 437A -0.10030
425A -> 437A 0.37366

425A -> 438A 0.28728
425A -> 439A 0.39142
425A -> 440A -0.10439
415B -> 438B -0.11039
417B -> 437B -0.10030
425B -> 437B 0.37366
425B -> 438B 0.28728
425B -> 439B 0.39142
425B -> 440B -0.10439

Excited State 136: 3.000-A 2.2936 eV 540.56 nm f=0.0000 <S**2>=2.000
406A -> 437A -0.13273
413A -> 437A -0.12780
417A -> 437A -0.24289
417A -> 438A 0.14874
418A -> 437A -0.26688
418A -> 438A 0.11066
418A -> 439A 0.14698
419A -> 437A -0.19827
419A -> 438A 0.11933
423A -> 438A -0.11548
406B -> 437B 0.13273
413B -> 437B 0.12780
417B -> 437B 0.24289
417B -> 438B -0.14874
418B -> 437B 0.26688
418B -> 438B -0.11066
418B -> 439B -0.14698
419B -> 437B 0.19827
419B -> 438B -0.11933
423B -> 438B 0.11548

Excited State 137: 1.000-A 2.2943 eV 540.39 nm f=0.0035 <S**2>=0.000
412A -> 437A -0.19640
412A -> 439A -0.14097
415A -> 437A -0.21111

415A -> 438A 0.15729
415A -> 439A -0.17983
415A -> 440A -0.16196
417A -> 437A 0.27114
417A -> 438A -0.10028
417A -> 439A 0.13144
420A -> 440A 0.15864
422A -> 437A 0.11527
425A -> 437A 0.12002
425A -> 439A 0.10681
412B -> 437B -0.19640
412B -> 439B -0.14097
415B -> 437B -0.21111
415B -> 438B 0.15729
415B -> 439B -0.17983
415B -> 440B -0.16196
417B -> 437B 0.27114
417B -> 438B -0.10028
417B -> 439B 0.13144
420B -> 440B 0.15864
422B -> 437B 0.11527
425B -> 437B 0.12002
425B -> 439B 0.10681

Excited State 138: 3.000-A 2.2999 eV 539.09 nm f=0.0000 <S**2>=2.000
410A -> 438A -0.10059
412A -> 437A -0.13077
415A -> 438A 0.14760
415A -> 440A -0.11254
417A -> 437A 0.14797
417A -> 438A 0.11942
418A -> 437A -0.25766
418A -> 438A -0.30052
420A -> 440A 0.15439
423A -> 438A -0.11082
410B -> 438B 0.10059

412B -> 437B 0.13077
415B -> 438B -0.14760
415B -> 440B 0.11254
417B -> 437B -0.14797
417B -> 438B -0.11942
418B -> 437B 0.25766
418B -> 438B 0.30052
420B -> 440B -0.15439
423B -> 438B 0.11082

Excited State 139: 1.000-A 2.3015 eV 538.71 nm f=0.0003 <S**2>=0.000
421A -> 437A 0.12939
422A -> 437A 0.51078
422A -> 438A -0.30972
422A -> 439A 0.20868
422A -> 440A 0.19166
421B -> 437B 0.12939
422B -> 437B 0.51078
422B -> 438B -0.30972
422B -> 439B 0.20868
422B -> 440B 0.19166

Excited State 140: 3.000-A 2.3018 eV 538.65 nm f=0.0000 <S**2>=2.000
421A -> 437A -0.12938
422A -> 437A -0.51936
422A -> 438A 0.31048
422A -> 439A -0.20803
422A -> 440A -0.19122
421B -> 437B 0.12938
422B -> 437B 0.51936
422B -> 438B -0.31048
422B -> 439B 0.20803
422B -> 440B 0.19122

Excited State 141: 3.000-A 2.3046 eV 537.98 nm f=0.0000 <S**2>=2.000
393A -> 437A 0.12301

405A -> 438A 0.11009
412A -> 438A 0.17253
412A -> 440A -0.14692
415A -> 437A -0.24588
415A -> 438A -0.10816
415A -> 439A -0.16353
417A -> 438A -0.19096
418A -> 437A -0.15116
418A -> 439A 0.10160
418A -> 440A -0.12159
393B -> 437B -0.12301
405B -> 438B -0.11009
412B -> 438B -0.17253
412B -> 440B 0.14692
415B -> 437B 0.24588
415B -> 438B 0.10816
415B -> 439B 0.16353
417B -> 438B 0.19096
418B -> 437B 0.15116
418B -> 439B -0.10160
418B -> 440B 0.12159

Excited State 142: 3.000-A 2.3057 eV 537.72 nm f=0.0000 <S**2>=2.000
406A -> 439A -0.11203
412A -> 437A 0.15646
412A -> 439A 0.12602
413A -> 437A 0.10447
414A -> 439A -0.11092
415A -> 437A 0.12451
415A -> 438A -0.11038
415A -> 439A 0.10557
415A -> 440A 0.12326
417A -> 440A -0.10126
418A -> 438A -0.32042
418A -> 440A -0.11274
420A -> 439A -0.16933

406B -> 439B 0.11203
412B -> 437B -0.15646
412B -> 439B -0.12602
413B -> 437B -0.10447
414B -> 439B 0.11092
415B -> 437B -0.12451
415B -> 438B 0.11038
415B -> 439B -0.10557
415B -> 440B -0.12326
417B -> 440B 0.10126
418B -> 438B 0.32042
418B -> 440B 0.11274
420B -> 439B 0.16933

Excited State 143: 3.000-A 2.3112 eV 536.45 nm f=0.0000 <S**2>=2.000
400A -> 437A -0.12160
411A -> 437A -0.11735
418A -> 439A -0.10564
419A -> 437A -0.38433
419A -> 438A 0.24278
420A -> 440A -0.12034
425A -> 438A -0.10209
400B -> 437B 0.12160
411B -> 437B 0.11735
418B -> 439B 0.10564
419B -> 437B 0.38433
419B -> 438B -0.24278
420B -> 440B 0.12034
425B -> 438B 0.10209

Excited State 144: 1.000-A 2.3124 eV 536.18 nm f=0.0024 <S**2>=0.000
418A -> 437A 0.39139
419A -> 437A 0.36068
420A -> 439A -0.25548
421A -> 437A -0.14183
418B -> 437B 0.39139

419B -> 437B 0.36068
420B -> 439B -0.25548
421B -> 437B -0.14183

Excited State 145: 3.000-A 2.3255 eV 533.15 nm f=0.0000 <S**2>=2.000
411A -> 438A -0.11824
412A -> 438A 0.13194
414A -> 439A 0.14175
414A -> 440A -0.12217
418A -> 437A -0.11216
418A -> 438A -0.23356
418A -> 439A -0.20844
418A -> 440A 0.19856
419A -> 438A -0.24877
419A -> 439A -0.11191
420A -> 439A 0.12886
420A -> 440A -0.11145
426A -> 440A -0.11805
411B -> 438B 0.11824
412B -> 438B -0.13194
414B -> 439B -0.14175
414B -> 440B 0.12217
418B -> 437B 0.11216
418B -> 438B 0.23356
418B -> 439B 0.20844
418B -> 440B -0.19856
419B -> 438B 0.24877
419B -> 439B 0.11191
420B -> 439B -0.12886
420B -> 440B 0.11145
426B -> 440B 0.11805

Excited State 146: 1.000-A 2.3279 eV 532.59 nm f=0.0009 <S**2>=0.000
424A -> 437A 0.41266
424A -> 439A 0.50933
424A -> 440A 0.14514

424B -> 437B 0.41266
424B -> 439B 0.50933
424B -> 440B 0.14514

Excited State 147: 3.000-A 2.3281 eV 532.56 nm f=0.0000 <S**2>=2.000
424A -> 437A 0.42065
424A -> 439A 0.51754
424A -> 440A 0.14494
424B -> 437B -0.42065
424B -> 439B -0.51754
424B -> 440B -0.14494

Excited State 148: 1.000-A 2.3310 eV 531.89 nm f=0.0103 <S**2>=0.000
414A -> 437A -0.13955
414A -> 438A -0.13133
414A -> 439A 0.14893
414A -> 440A -0.13790
418A -> 437A -0.23443
419A -> 437A 0.14910
419A -> 438A 0.20836
419A -> 439A -0.13085
419A -> 440A 0.12415
420A -> 440A 0.31025
414B -> 437B -0.13955
414B -> 438B -0.13133
414B -> 439B 0.14893
414B -> 440B -0.13790
418B -> 437B -0.23443
419B -> 437B 0.14910
419B -> 438B 0.20836
419B -> 439B -0.13085
419B -> 440B 0.12415
420B -> 440B 0.31025

Excited State 149: 1.000-A 2.3337 eV 531.28 nm f=0.0029 <S**2>=0.000
412A -> 437A -0.16502

413A -> 437A -0.10318
415A -> 438A 0.10833
415A -> 440A -0.10163
416A -> 437A -0.12795
417A -> 438A 0.10134
418A -> 437A 0.11125
418A -> 438A 0.23789
419A -> 437A -0.18669
419A -> 438A 0.38786
420A -> 439A -0.12704
424A -> 439A 0.10752
425A -> 440A 0.10747
412B -> 437B -0.16502
413B -> 437B -0.10318
415B -> 438B 0.10833
415B -> 440B -0.10163
416B -> 437B -0.12795
417B -> 438B 0.10134
418B -> 437B 0.11125
418B -> 438B 0.23789
419B -> 437B -0.18669
419B -> 438B 0.38786
420B -> 439B -0.12704
424B -> 439B 0.10752
425B -> 440B 0.10747

Excited State 150: 3.000-A 2.3376 eV 530.38 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.15082
395A -> 438A 0.11144
400A -> 437A -0.11466
402A -> 439A 0.10111
413A -> 437A 0.15103
415A -> 437A 0.10192
418A -> 437A -0.10273
423A -> 437A 0.11156
423A -> 439A -0.10934

425A -> 438A 0.16312
425A -> 439A -0.14103
425A -> 440A -0.27014
395B -> 437B 0.15082
395B -> 438B -0.11144
400B -> 437B 0.11466
402B -> 439B -0.10111
413B -> 437B -0.15103
415B -> 437B -0.10192
418B -> 437B 0.10273
423B -> 437B -0.11156
423B -> 439B 0.10934
425B -> 438B -0.16312
425B -> 439B 0.14103
425B -> 440B 0.27014

Excited State 151: 3.000-A 2.3396 eV 529.94 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.11828
423A -> 437A -0.16014
423A -> 438A 0.11473
423A -> 439A 0.19584
423A -> 440A 0.11178
425A -> 438A 0.25927
425A -> 439A -0.20045
425A -> 440A -0.37630
395B -> 437B -0.11828
423B -> 437B 0.16014
423B -> 438B -0.11473
423B -> 439B -0.19584
423B -> 440B -0.11178
425B -> 438B -0.25927
425B -> 439B 0.20045
425B -> 440B 0.37630

Excited State 152: 1.000-A 2.3396 eV 529.93 nm f=0.0055 <S**2>=0.000
418A -> 438A -0.30097

418A -> 439A -0.11562
419A -> 439A -0.10999
423A -> 437A -0.16809
423A -> 438A 0.12479
423A -> 439A 0.18709
425A -> 438A -0.20090
425A -> 439A 0.16943
425A -> 440A 0.30358
418B -> 438B -0.30097
418B -> 439B -0.11562
419B -> 439B -0.10999
423B -> 437B -0.16809
423B -> 438B 0.12479
423B -> 439B 0.18709
425B -> 438B -0.20090
425B -> 439B 0.16943
425B -> 440B 0.30358

Excited State 153: 1.000-A 2.3404 eV 529.77 nm f=0.0124 <S**2>=0.000
412A -> 437A 0.14055
412A -> 439A 0.10742
415A -> 437A 0.13446
416A -> 437A -0.11025
417A -> 437A 0.26621
418A -> 439A -0.14078
420A -> 438A -0.10755
423A -> 437A -0.18748
423A -> 438A 0.12765
423A -> 439A 0.23599
423A -> 440A 0.12497
425A -> 440A -0.16951
412B -> 437B 0.14055
412B -> 439B 0.10742
415B -> 437B 0.13446
416B -> 437B -0.11025
417B -> 437B 0.26621

418B -> 439B -0.14078
420B -> 438B -0.10755
423B -> 437B -0.18748
423B -> 438B 0.12765
423B -> 439B 0.23599
423B -> 440B 0.12497
425B -> 440B -0.16951

Excited State 154: 1.000-A 2.3436 eV 529.04 nm f=0.0104 <S**2>=0.000
412A -> 437A 0.12809
417A -> 437A 0.24305
420A -> 438A -0.13652
423A -> 437A 0.17212
423A -> 438A -0.13409
423A -> 439A -0.21802
423A -> 440A -0.11195
425A -> 438A -0.19797
425A -> 439A 0.16837
425A -> 440A 0.31032
412B -> 437B 0.12809
417B -> 437B 0.24305
420B -> 438B -0.13652
423B -> 437B 0.17212
423B -> 438B -0.13409
423B -> 439B -0.21802
423B -> 440B -0.11195
425B -> 438B -0.19797
425B -> 439B 0.16837
425B -> 440B 0.31032

Excited State 155: 3.000-A 2.3446 eV 528.82 nm f=0.0000 <S**2>=2.000
395A -> 437A 0.10506
423A -> 437A 0.32691
423A -> 438A -0.23892
423A -> 439A -0.37447
423A -> 440A -0.18466

425A -> 440A -0.10137
395B -> 437B -0.10506
423B -> 437B -0.32691
423B -> 438B 0.23892
423B -> 439B 0.37447
423B -> 440B 0.18466
425B -> 440B 0.10137

Excited State 156: 1.000-A 2.3475 eV 528.15 nm f=0.0087 <S**2>=0.000
416A -> 437A 0.10954
416A -> 438A -0.10644
418A -> 438A 0.24664
419A -> 437A 0.16530
419A -> 438A -0.11026
419A -> 440A -0.13970
420A -> 439A 0.14851
420A -> 440A 0.14309
423A -> 437A -0.21612
423A -> 438A 0.15670
423A -> 439A 0.24271
423A -> 440A 0.12668
425A -> 440A 0.16916
416B -> 437B 0.10954
416B -> 438B -0.10644
418B -> 438B 0.24664
419B -> 437B 0.16530
419B -> 438B -0.11026
419B -> 440B -0.13970
420B -> 439B 0.14851
420B -> 440B 0.14309
423B -> 437B -0.21612
423B -> 438B 0.15670
423B -> 439B 0.24271
423B -> 440B 0.12668
425B -> 440B 0.16916

Excited State 157: 1.000-A 2.3499 eV 527.62 nm f=0.0108 <S**2>=0.000

| | |
|---|---|
| 410A -> 437A | -0.12540 |
| 412A -> 438A | 0.14752 |
| 415A -> 437A | -0.11014 |
| 415A -> 438A | -0.12967 |
| 417A -> 438A | 0.37584 |
| 417A -> 440A | -0.15318 |
| 418A -> 438A | -0.23920 |
| 418A -> 439A | 0.15499 |
| 419A -> 438A | 0.10421 |
| 420A -> 437A | -0.12816 |
| 420A -> 438A | -0.12021 |
| 420A -> 440A | 0.10886 |
| 410B -> 437B | -0.12540 |
| 412B -> 438B | 0.14752 |
| 415B -> 437B | -0.11014 |
| 415B -> 438B | -0.12967 |
| 417B -> 438B | 0.37584 |
| 417B -> 440B | -0.15318 |
| 418B -> 438B | -0.23920 |
| 418B -> 439B | 0.15499 |
| 419B -> 438B | 0.10421 |
| 420B -> 437B | -0.12816 |
| 420B -> 438B | -0.12021 |
| 420B -> 440B | 0.10886 |

Excited State 158: 3.000-A 2.3513 eV 527.30 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 406A -> 438A | 0.10488 |
| 406A -> 439A | -0.13228 |
| 406A -> 440A | 0.11315 |
| 409A -> 439A | 0.11135 |
| 413A -> 437A | -0.16568 |
| 413A -> 438A | -0.17906 |
| 413A -> 439A | 0.12983 |
| 413A -> 440A | -0.14757 |
| 414A -> 437A | 0.13134 |

414A -> 438A 0.17592
414A -> 439A -0.18882
414A -> 440A 0.17113
419A -> 437A -0.10186
419A -> 438A -0.19072
420A -> 440A -0.13545
406B -> 438B -0.10488
406B -> 439B 0.13228
406B -> 440B -0.11315
409B -> 439B -0.11135
413B -> 437B 0.16568
413B -> 438B 0.17906
413B -> 439B -0.12983
413B -> 440B 0.14757
414B -> 437B -0.13134
414B -> 438B -0.17592
414B -> 439B 0.18882
414B -> 440B -0.17113
419B -> 437B 0.10186
419B -> 438B 0.19072
420B -> 440B 0.13545

Excited State 159: 3.000-A 2.3575 eV 525.92 nm f=0.0000 <S**2>=2.000
395A -> 437A -0.10254
395A -> 439A 0.11038
413A -> 437A -0.19437
413A -> 438A 0.15543
416A -> 437A -0.21936
416A -> 438A 0.13797
418A -> 437A 0.15959
418A -> 438A -0.16660
420A -> 439A -0.20198
420A -> 440A -0.16682
395B -> 437B 0.10254
395B -> 439B -0.11038
413B -> 437B 0.19437

413B -> 438B -0.15543
416B -> 437B 0.21936
416B -> 438B -0.13797
418B -> 437B -0.15959
418B -> 438B 0.16660
420B -> 439B 0.20198
420B -> 440B 0.16682

Excited State 160: 3.000-A 2.3603 eV 525.28 nm f=0.0000 <S**2>=2.000
409A -> 437A 0.10113
413A -> 438A -0.11120
413A -> 439A -0.22189
417A -> 437A -0.16368
417A -> 439A -0.12483
418A -> 438A 0.11035
418A -> 440A -0.20026
419A -> 439A -0.29449
419A -> 440A -0.11290
420A -> 438A 0.13985
425A -> 439A -0.11433
425A -> 440A -0.12673
409B -> 437B -0.10113
413B -> 438B 0.11120
413B -> 439B 0.22189
417B -> 437B 0.16368
417B -> 439B 0.12483
418B -> 438B -0.11035
418B -> 440B 0.20026
419B -> 439B 0.29449
419B -> 440B 0.11290
420B -> 438B -0.13985
425B -> 439B 0.11433
425B -> 440B 0.12673

Excited State 161: 3.000-A 2.3713 eV 522.85 nm f=0.0000 <S**2>=2.000
409A -> 438A -0.11523

413A -> 438A 0.17706
413A -> 440A -0.12570
417A -> 438A 0.23887
417A -> 439A -0.14453
418A -> 439A -0.25828
419A -> 438A 0.15766
419A -> 439A -0.12196
419A -> 440A -0.12834
420A -> 439A -0.10105
420A -> 440A 0.18122
421A -> 438A -0.10951
425A -> 440A -0.11122
409B -> 438B 0.11523
413B -> 438B -0.17706
413B -> 440B 0.12570
417B -> 438B -0.23887
417B -> 439B 0.14453
418B -> 439B 0.25828
419B -> 438B -0.15766
419B -> 439B 0.12196
419B -> 440B 0.12834
420B -> 439B 0.10105
420B -> 440B -0.18122
421B -> 438B 0.10951
425B -> 440B 0.11122

Excited State 162: 1.000-A 2.3774 eV 521.52 nm f=0.0084 <S**2>=0.000
413A -> 437A 0.12670
417A -> 438A -0.22512
417A -> 439A 0.12473
418A -> 439A 0.40095
418A -> 440A -0.11994
419A -> 439A 0.27869
420A -> 440A -0.13345
421A -> 439A -0.14776
413B -> 437B 0.12670

417B -> 438B -0.22512
417B -> 439B 0.12473
418B -> 439B 0.40095
418B -> 440B -0.11994
419B -> 439B 0.27869
420B -> 440B -0.13345
421B -> 439B -0.14776

Excited State 163: 3.000-A 2.3782 eV 521.33 nm f=0.0000 <S**2>=2.000
408A -> 439A 0.10854
411A -> 439A -0.12304
413A -> 439A 0.11208
413A -> 440A 0.20993
418A -> 439A -0.29648
419A -> 439A -0.10691
419A -> 440A 0.11409
420A -> 437A 0.19045
421A -> 439A 0.17989
426A -> 440A -0.16460
408B -> 439B -0.10854
411B -> 439B 0.12304
413B -> 439B -0.11208
413B -> 440B -0.20993
418B -> 439B 0.29648
419B -> 439B 0.10691
419B -> 440B -0.11409
420B -> 437B -0.19045
421B -> 439B -0.17989
426B -> 440B 0.16460

Excited State 164: 3.000-A 2.3888 eV 519.03 nm f=0.0000 <S**2>=2.000
411A -> 440A -0.12325
413A -> 439A 0.13224
417A -> 440A -0.13486
418A -> 438A -0.11292
418A -> 440A -0.39126

419A -> 440A -0.26768
420A -> 438A -0.14851
421A -> 440A 0.19352
426A -> 439A -0.16310
411B -> 440B 0.12325
413B -> 439B -0.13224
417B -> 440B 0.13486
418B -> 438B 0.11292
418B -> 440B 0.39126
419B -> 440B 0.26768
420B -> 438B 0.14851
421B -> 440B -0.19352
426B -> 439B 0.16310

Excited State 165: 3.000-A 2.3930 eV 518.10 nm f=0.0000 <S**2>=2.000
422A -> 439A -0.17561
424A -> 438A -0.34120
424A -> 439A -0.10605
424A -> 440A 0.49068
422B -> 439B 0.17561
424B -> 438B 0.34120
424B -> 439B 0.10605
424B -> 440B -0.49068

Excited State 166: 1.000-A 2.3932 eV 518.06 nm f=0.0002 <S**2>=0.000
424A -> 438A -0.38773
424A -> 439A -0.12137
424A -> 440A 0.56128
424B -> 438B -0.38773
424B -> 439B -0.12137
424B -> 440B 0.56128

Excited State 167: 3.000-A 2.3938 eV 517.94 nm f=0.0000 <S**2>=2.000
421A -> 439A -0.13915
422A -> 437A 0.22137
422A -> 438A 0.14485

422A -> 439A -0.51417
422A -> 440A 0.19162
424A -> 438A 0.15120
424A -> 440A -0.21743
421B -> 439B 0.13915
422B -> 437B -0.22137
422B -> 438B -0.14485
422B -> 439B 0.51417
422B -> 440B -0.19162
424B -> 438B -0.15120
424B -> 440B 0.21743

Excited State 168: 1.000-A 2.3940 eV 517.90 nm f=0.0002 <S**2>=0.000
421A -> 439A 0.13566
422A -> 437A -0.24276
422A -> 438A -0.14967
422A -> 439A 0.57499
422A -> 440A -0.21896
421B -> 439B 0.13566
422B -> 437B -0.24276
422B -> 438B -0.14967
422B -> 439B 0.57499
422B -> 440B -0.21896

Excited State 169: 3.000-A 2.3953 eV 517.62 nm f=0.0000 <S**2>=2.000
391A -> 438A -0.11402
393A -> 437A 0.10745
393A -> 438A 0.17900
393A -> 440A -0.11917
394A -> 438A -0.11446
409A -> 437A 0.11612
409A -> 438A 0.13144
409A -> 440A -0.10756
412A -> 437A -0.13668
412A -> 438A -0.13926
419A -> 437A 0.10698

419A -> 438A 0.10477
419A -> 439A 0.11691
422A -> 439A -0.18929
424A -> 438A -0.11163
424A -> 440A 0.15814
391B -> 438B 0.11402
393B -> 437B -0.10745
393B -> 438B -0.17900
393B -> 440B 0.11917
394B -> 438B 0.11446
409B -> 437B -0.11612
409B -> 438B -0.13144
409B -> 440B 0.10756
412B -> 437B 0.13668
412B -> 438B 0.13926
419B -> 437B -0.10698
419B -> 438B -0.10477
419B -> 439B -0.11691
422B -> 439B 0.18929
424B -> 438B 0.11163
424B -> 440B -0.15814

Excited State 170: 1.000-A 2.4027 eV 516.03 nm f=0.0140 <S**2>=0.000
411A -> 438A -0.10108
413A -> 437A -0.20171
413A -> 439A 0.14828
417A -> 439A 0.23062
417A -> 440A 0.16517
418A -> 440A 0.33467
419A -> 440A 0.30410
411B -> 438B -0.10108
413B -> 437B -0.20171
413B -> 439B 0.14828
417B -> 439B 0.23062
417B -> 440B 0.16517
418B -> 440B 0.33467

419B -> 440B 0.30410

Excited State 171: 1.000-A 2.4043 eV 515.68 nm f=0.0093 <S**2>=0.000
413A -> 437A 0.29678
414A -> 437A 0.14108
414A -> 439A -0.11400
416A -> 437A 0.11136
417A -> 439A -0.20436
418A -> 439A -0.10446
418A -> 440A 0.34854
419A -> 437A 0.14590
419A -> 439A 0.20202
413B -> 437B 0.29678
414B -> 437B 0.14108
414B -> 439B -0.11400
416B -> 437B 0.11136
417B -> 439B -0.20436
418B -> 439B -0.10446
418B -> 440B 0.34854
419B -> 437B 0.14590
419B -> 439B 0.20202

Excited State 172: 1.000-A 2.4091 eV 514.66 nm f=0.0003 <S**2>=0.000
411A -> 437A -0.11324
413A -> 438A -0.19340
413A -> 439A -0.16420
417A -> 437A 0.23203
417A -> 439A -0.18816
418A -> 438A 0.12556
418A -> 439A 0.26274
418A -> 440A 0.17232
419A -> 437A -0.11428
419A -> 438A -0.17707
419A -> 439A -0.21886
419A -> 440A 0.14184
421A -> 440A -0.12582

411B -> 437B -0.11324
413B -> 438B -0.19340
413B -> 439B -0.16420
417B -> 437B 0.23203
417B -> 439B -0.18816
418B -> 438B 0.12556
418B -> 439B 0.26274
418B -> 440B 0.17232
419B -> 437B -0.11428
419B -> 438B -0.17707
419B -> 439B -0.21886
419B -> 440B 0.14184
421B -> 440B -0.12582

Excited State 173: 1.000-A 2.4170 eV 512.96 nm f=0.0050 <S**2>=0.000
406A -> 438A 0.10420
406A -> 439A -0.10546
406A -> 440A 0.11198
408A -> 439A 0.10513
411A -> 437A 0.16288
411A -> 439A -0.11999
413A -> 438A 0.15201
413A -> 440A 0.10922
414A -> 438A 0.18604
414A -> 439A -0.14272
414A -> 440A 0.14507
416A -> 438A 0.11838
416A -> 439A -0.12818
416A -> 440A 0.11740
417A -> 438A 0.10482
417A -> 440A 0.20968
419A -> 437A -0.11533
406B -> 438B 0.10420
406B -> 439B -0.10546
406B -> 440B 0.11198
408B -> 439B 0.10513

411B -> 437B 0.16288
411B -> 439B -0.11999
413B -> 438B 0.15201
413B -> 440B 0.10922
414B -> 438B 0.18604
414B -> 439B -0.14272
414B -> 440B 0.14507
416B -> 438B 0.11838
416B -> 439B -0.12818
416B -> 440B 0.11740
417B -> 438B 0.10482
417B -> 440B 0.20968
419B -> 437B -0.11533

Excited State 174: 3.000-A 2.4181 eV 512.73 nm f=0.0000 <S**2>=2.000
392A -> 437A 0.14568
392A -> 439A 0.12954
392A -> 440A 0.11247
393A -> 437A -0.17997
393A -> 439A -0.14626
394A -> 438A 0.11103
394A -> 440A -0.10921
395A -> 437A -0.12084
407A -> 437A 0.12051
412A -> 437A -0.10118
415A -> 437A -0.12712
417A -> 437A -0.21148
418A -> 439A -0.13994
419A -> 437A 0.13828
419A -> 439A 0.20371
392B -> 437B -0.14568
392B -> 439B -0.12954
392B -> 440B -0.11247
393B -> 437B 0.17997
393B -> 439B 0.14626
394B -> 438B -0.11103

394B -> 440B 0.10921
395B -> 437B 0.12084
407B -> 437B -0.12051
412B -> 437B 0.10118
415B -> 437B 0.12712
417B -> 437B 0.21148
418B -> 439B 0.13994
419B -> 437B -0.13828
419B -> 439B -0.20371

Excited State 175: 3.000-A 2.4250 eV 511.28 nm f=0.0000 <S**2>=2.000
392A -> 437A 0.11036
395A -> 439A -0.10416
417A -> 437A 0.25013
417A -> 438A -0.10336
417A -> 439A -0.25903
418A -> 439A 0.11387
422A -> 438A -0.16130
422A -> 440A -0.26902
392B -> 437B -0.11036
395B -> 439B 0.10416
417B -> 437B -0.25013
417B -> 438B 0.10336
417B -> 439B 0.25903
418B -> 439B -0.11387
422B -> 438B 0.16130
422B -> 440B 0.26902

Excited State 176: 1.000-A 2.4289 eV 510.45 nm f=0.0001 <S**2>=0.000
421A -> 440A 0.11742
422A -> 437A -0.10749
422A -> 438A 0.31653
422A -> 439A 0.23618
422A -> 440A 0.54144
421B -> 440B 0.11742
422B -> 437B -0.10749

422B -> 438B 0.31653
422B -> 439B 0.23618
422B -> 440B 0.54144

Excited State 177: 3.000-A 2.4290 eV 510.43 nm f=0.0000 <S**2>=2.000
417A -> 437A -0.14681
421A -> 440A -0.10471
422A -> 438A -0.26403
422A -> 439A -0.21604
422A -> 440A -0.44668
417B -> 437B 0.14681
421B -> 440B 0.10471
422B -> 438B 0.26403
422B -> 439B 0.21604
422B -> 440B 0.44668

Excited State 178: 3.000-A 2.4309 eV 510.04 nm f=0.0000 <S**2>=2.000
421A -> 440A 0.12288
423A -> 438A -0.19814
423A -> 439A 0.35760
423A -> 440A -0.53220
421B -> 440B -0.12288
423B -> 438B 0.19814
423B -> 439B -0.35760
423B -> 440B 0.53220

Excited State 179: 1.000-A 2.4310 eV 510.01 nm f=0.0000 <S**2>=0.000
421A -> 440A -0.13993
423A -> 438A 0.19861
423A -> 439A -0.35245
423A -> 440A 0.53247
421B -> 440B -0.13993
423B -> 438B 0.19861
423B -> 439B -0.35245
423B -> 440B 0.53247

Excited State 180: 3.000-A 2.4346 eV 509.25 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 393A -> 438A | -0.13434 |
| 393A -> 440A | 0.12765 |
| 417A -> 438A | -0.23057 |
| 417A -> 439A | -0.20429 |
| 417A -> 440A | -0.12700 |
| 418A -> 437A | -0.13250 |
| 419A -> 437A | 0.18243 |
| 419A -> 438A | 0.17673 |
| 419A -> 440A | -0.13561 |
| 420A -> 440A | -0.11539 |
| 422A -> 440A | 0.13601 |
| 393B -> 438B | 0.13434 |
| 393B -> 440B | -0.12765 |
| 417B -> 438B | 0.23057 |
| 417B -> 439B | 0.20429 |
| 417B -> 440B | 0.12700 |
| 418B -> 437B | 0.13250 |
| 419B -> 437B | -0.18243 |
| 419B -> 438B | -0.17673 |
| 419B -> 440B | 0.13561 |
| 420B -> 440B | 0.11539 |
| 422B -> 440B | -0.13601 |

Excited State 181: 1.000-A 2.4452 eV 507.06 nm f=0.0021 <S**2>=0.000

| | |
|---|---|
| 407A -> 437A | 0.11066 |
| 413A -> 437A | 0.15946 |
| 413A -> 438A | -0.24473 |
| 413A -> 440A | 0.16805 |
| 416A -> 438A | -0.11873 |
| 417A -> 437A | -0.13867 |
| 417A -> 438A | 0.11678 |
| 418A -> 439A | -0.11223 |
| 418A -> 440A | -0.18266 |
| 419A -> 438A | -0.13983 |
| 419A -> 439A | 0.17053 |

419A -> 440A 0.34618
407B -> 437B 0.11066
413B -> 437B 0.15946
413B -> 438B -0.24473
413B -> 440B 0.16805
416B -> 438B -0.11873
417B -> 437B -0.13867
417B -> 438B 0.11678
418B -> 439B -0.11223
418B -> 440B -0.18266
419B -> 438B -0.13983
419B -> 439B 0.17053
419B -> 440B 0.34618

Excited State 182: 3.000-A 2.4502 eV 506.01 nm f=0.0000 <S**2>=2.000
411A -> 439A 0.16029
413A -> 440A 0.12770
416A -> 437A 0.15356
416A -> 438A 0.22356
416A -> 439A -0.15903
416A -> 440A 0.18508
417A -> 438A 0.21327
417A -> 439A -0.28175
417A -> 440A 0.18110
419A -> 438A -0.10852
419A -> 439A 0.18545
411B -> 439B -0.16029
413B -> 440B -0.12770
416B -> 437B -0.15356
416B -> 438B -0.22356
416B -> 439B 0.15903
416B -> 440B -0.18508
417B -> 438B -0.21327
417B -> 439B 0.28175
417B -> 440B -0.18110
419B -> 438B 0.10852

419B -> 439B -0.18545

Excited State 183: 1.000-A 2.4596 eV 504.07 nm f=0.0025 <S**2>=0.000
411A -> 437A -0.12158
411A -> 438A -0.14921
411A -> 439A 0.15818
411A -> 440A -0.12575
413A -> 438A 0.10427
416A -> 437A 0.16272
416A -> 438A 0.25378
416A -> 439A -0.16877
416A -> 440A 0.20188
417A -> 438A 0.18342
417A -> 439A -0.14680
417A -> 440A 0.21408
411B -> 437B -0.12158
411B -> 438B -0.14921
411B -> 439B 0.15818
411B -> 440B -0.12575
413B -> 438B 0.10427
416B -> 437B 0.16272
416B -> 438B 0.25378
416B -> 439B -0.16877
416B -> 440B 0.20188
417B -> 438B 0.18342
417B -> 439B -0.14680
417B -> 440B 0.21408

Excited State 184: 3.000-A 2.4611 eV 503.77 nm f=0.0000 <S**2>=2.000
416A -> 437A -0.16226
416A -> 438A -0.31431
416A -> 439A 0.14623
416A -> 440A -0.11939
417A -> 438A 0.11761
417A -> 439A -0.13649
417A -> 440A -0.14880

418A -> 440A -0.17779
419A -> 438A -0.13800
419A -> 440A 0.28689
416B -> 437B 0.16226
416B -> 438B 0.31431
416B -> 439B -0.14623
416B -> 440B 0.11939
417B -> 438B -0.11761
417B -> 439B 0.13649
417B -> 440B 0.14880
418B -> 440B 0.17779
419B -> 438B 0.13800
419B -> 440B -0.28689

Excited State 185: 1.000-A 2.4653 eV 502.91 nm f=0.0015 <S**2>=0.000
413A -> 438A -0.21349
413A -> 440A -0.12412
414A -> 438A -0.10942
416A -> 437A 0.19888
416A -> 438A 0.29937
416A -> 439A -0.19946
416A -> 440A 0.20303
417A -> 438A -0.12410
417A -> 439A 0.15722
417A -> 440A -0.20072
418A -> 440A 0.14265
413B -> 438B -0.21349
413B -> 440B -0.12412
414B -> 438B -0.10942
416B -> 437B 0.19888
416B -> 438B 0.29937
416B -> 439B -0.19946
416B -> 440B 0.20303
417B -> 438B -0.12410
417B -> 439B 0.15722
417B -> 440B -0.20072

418B -> 440B 0.14265

Excited State 186: 3.000-A 2.4655 eV 502.88 nm f=0.0000 <S**2>=2.000
413A -> 439A 0.12236
416A -> 437A 0.14408
416A -> 438A 0.17447
416A -> 439A -0.15038
416A -> 440A 0.16638
417A -> 438A -0.10477
417A -> 439A 0.13778
417A -> 440A -0.35488
418A -> 438A 0.14915
418A -> 439A -0.11311
419A -> 438A -0.15823
413B -> 439B -0.12236
416B -> 437B -0.14408
416B -> 438B -0.17447
416B -> 439B 0.15038
416B -> 440B -0.16638
417B -> 438B 0.10477
417B -> 439B -0.13778
417B -> 440B 0.35488
418B -> 438B -0.14915
418B -> 439B 0.11311
419B -> 438B 0.15823

Excited State 187: 1.000-A 2.4747 eV 501.01 nm f=0.0077 <S**2>=0.000
407A -> 439A -0.11903
409A -> 439A -0.11285
411A -> 439A -0.10152
413A -> 437A 0.36373
417A -> 439A 0.30259
418A -> 437A 0.10442
419A -> 437A -0.15786
419A -> 439A -0.15722
407B -> 439B -0.11903

409B -> 439B -0.11285
411B -> 439B -0.10152
413B -> 437B 0.36373
417B -> 439B 0.30259
418B -> 437B 0.10442
419B -> 437B -0.15786
419B -> 439B -0.15722

Excited State 188: 3.000-A 2.4824 eV 499.46 nm f=0.0000 <S**2>=2.000
411A -> 437A -0.34042
411A -> 438A 0.19659
411A -> 439A 0.11175
413A -> 437A -0.24160
413A -> 438A 0.19731
414A -> 437A 0.10672
415A -> 437A 0.16720
415A -> 438A -0.11394
416A -> 438A -0.11915
417A -> 439A 0.10945
417A -> 440A 0.10685
419A -> 437A 0.12995
411B -> 437B 0.34042
411B -> 438B -0.19659
411B -> 439B -0.11175
413B -> 437B 0.24160
413B -> 438B -0.19731
414B -> 437B -0.10672
415B -> 437B -0.16720
415B -> 438B 0.11394
416B -> 438B 0.11915
417B -> 439B -0.10945
417B -> 440B -0.10685
419B -> 437B -0.12995

Excited State 189: 1.000-A 2.4867 eV 498.59 nm f=0.0135 <S**2>=0.000
403A -> 437A -0.12887

406A -> 439A 0.11237
411A -> 437A 0.36189
411A -> 438A -0.16656
413A -> 438A -0.15590
413A -> 439A -0.17650
414A -> 437A -0.16646
415A -> 437A -0.15692
415A -> 438A 0.10313
417A -> 439A -0.17189
419A -> 438A 0.10806
403B -> 437B -0.12887
406B -> 439B 0.11237
411B -> 437B 0.36189
411B -> 438B -0.16656
413B -> 438B -0.15590
413B -> 439B -0.17650
414B -> 437B -0.16646
415B -> 437B -0.15692
415B -> 438B 0.10313
417B -> 439B -0.17189
419B -> 438B 0.10806

Excited State 190: 1.000-A 2.4950 eV 496.93 nm f=0.0199 <S**2>=0.000
399A -> 438A 0.10864
402A -> 437A 0.11476
402A -> 438A 0.10514
404A -> 437A -0.14393
405A -> 438A -0.16761
406A -> 438A 0.16636
409A -> 437A 0.22496
409A -> 438A 0.10750
409A -> 440A -0.12143
410A -> 437A -0.12952
412A -> 438A -0.11129
413A -> 437A -0.13442
413A -> 438A -0.10703

417A -> 440A 0.17104
399B -> 438B 0.10864
402B -> 437B 0.11476
402B -> 438B 0.10514
404B -> 437B -0.14393
405B -> 438B -0.16761
406B -> 438B 0.16636
409B -> 437B 0.22496
409B -> 438B 0.10750
409B -> 440B -0.12143
410B -> 437B -0.12952
412B -> 438B -0.11129
413B -> 437B -0.13442
413B -> 438B -0.10703
417B -> 440B 0.17104

Excited State 191: 1.000-A 2.4975 eV 496.43 nm f=0.0015 <S**2>=0.000
402A -> 438A -0.10618
403A -> 439A 0.13393
404A -> 438A 0.15633
405A -> 437A 0.21319
406A -> 437A -0.13598
409A -> 438A -0.15230
410A -> 437A 0.15695
412A -> 437A 0.15774
412A -> 438A 0.12438
413A -> 437A -0.12206
413A -> 438A -0.11554
413A -> 439A -0.10070
416A -> 439A -0.10471
417A -> 440A 0.11402
419A -> 437A 0.11776
419A -> 440A -0.10946
402B -> 438B -0.10618
403B -> 439B 0.13393
404B -> 438B 0.15633

405B -> 437B 0.21319
406B -> 437B -0.13598
409B -> 438B -0.15230
410B -> 437B 0.15695
412B -> 437B 0.15774
412B -> 438B 0.12438
413B -> 437B -0.12206
413B -> 438B -0.11554
413B -> 439B -0.10070
416B -> 439B -0.10471
417B -> 440B 0.11402
419B -> 437B 0.11776
419B -> 440B -0.10946

Excited State 192: 1.000-A 2.5047 eV 495.01 nm f=0.0107 <S**2>=0.000
400A -> 439A -0.10055
403A -> 437A 0.21895
403A -> 438A -0.11113
404A -> 439A -0.13742
405A -> 439A 0.12851
406A -> 437A -0.10218
406A -> 439A -0.11349
406A -> 440A -0.10761
407A -> 437A -0.11753
409A -> 437A -0.10085
410A -> 437A -0.10267
411A -> 437A 0.11019
411A -> 438A -0.11222
412A -> 437A 0.16675
412A -> 439A 0.10116
413A -> 437A 0.11669
413A -> 438A -0.15381
415A -> 438A 0.10987
416A -> 437A -0.11805
417A -> 439A -0.10992
400B -> 439B -0.10055

403B -> 437B 0.21895
403B -> 438B -0.11113
404B -> 439B -0.13742
405B -> 439B 0.12851
406B -> 437B -0.10218
406B -> 439B -0.11349
406B -> 440B -0.10761
407B -> 437B -0.11753
409B -> 437B -0.10085
410B -> 437B -0.10267
411B -> 437B 0.11019
411B -> 438B -0.11222
412B -> 437B 0.16675
412B -> 439B 0.10116
413B -> 437B 0.11669
413B -> 438B -0.15381
415B -> 438B 0.10987
416B -> 437B -0.11805
417B -> 439B -0.10992

Excited State 193: 3.000-A 2.5099 eV 493.97 nm f=0.0000 <S**2>=2.000
409A -> 440A 0.10179
410A -> 437A -0.26224
410A -> 438A -0.18779
410A -> 439A -0.15367
410A -> 440A 0.16095
411A -> 437A -0.13910
411A -> 438A -0.25828
413A -> 437A 0.10725
413A -> 438A 0.19301
414A -> 437A 0.11608
414A -> 438A 0.18572
415A -> 438A 0.13902
417A -> 438A -0.16723
418A -> 438A 0.10673
409B -> 440B -0.10179

410B -> 437B 0.26224
410B -> 438B 0.18779
410B -> 439B 0.15367
410B -> 440B -0.16095
411B -> 437B 0.13910
411B -> 438B 0.25828
413B -> 437B -0.10725
413B -> 438B -0.19301
414B -> 437B -0.11608
414B -> 438B -0.18572
415B -> 438B -0.13902
417B -> 438B 0.16723
418B -> 438B -0.10673

Excited State 194: 1.000-A 2.5139 eV 493.19 nm f=0.0039 <S**2>=0.000
404A -> 437A 0.14958
405A -> 438A 0.11878
409A -> 437A -0.14218
410A -> 437A -0.28494
411A -> 437A -0.20093
411A -> 439A -0.11007
412A -> 438A 0.11573
413A -> 438A -0.19291
417A -> 440A 0.28624
419A -> 438A 0.14207
419A -> 440A -0.15470
404B -> 437B 0.14958
405B -> 438B 0.11878
409B -> 437B -0.14218
410B -> 437B -0.28494
411B -> 437B -0.20093
411B -> 439B -0.11007
412B -> 438B 0.11573
413B -> 438B -0.19291
417B -> 440B 0.28624
419B -> 438B 0.14207

419B -> 440B -0.15470

Excited State 195: 1.000-A 2.5234 eV 491.34 nm f=0.0040 <S**2>=0.000
405A -> 437A -0.10333
406A -> 437A 0.15287
410A -> 437A 0.30758
410A -> 438A 0.13781
410A -> 439A 0.16791
411A -> 438A 0.13284
413A -> 438A -0.28328
414A -> 438A -0.15491
417A -> 438A 0.16069
417A -> 440A 0.13693
418A -> 438A -0.11032
405B -> 437B -0.10333
406B -> 437B 0.15287
410B -> 437B 0.30758
410B -> 438B 0.13781
410B -> 439B 0.16791
411B -> 438B 0.13284
413B -> 438B -0.28328
414B -> 438B -0.15491
417B -> 438B 0.16069
417B -> 440B 0.13693
418B -> 438B -0.11032

Excited State 196: 3.000-A 2.5236 eV 491.30 nm f=0.0000 <S**2>=2.000
391A -> 438A -0.10181
391A -> 439A 0.10769
407A -> 437A 0.13646
409A -> 438A -0.17100
410A -> 437A -0.33392
410A -> 440A -0.12359
411A -> 438A 0.10774
411A -> 439A -0.12000
413A -> 437A -0.14569

413A -> 440A -0.11072
414A -> 437A -0.12883
417A -> 440A 0.16051
418A -> 440A -0.10013
419A -> 440A 0.11360
391B -> 438B 0.10181
391B -> 439B -0.10769
407B -> 437B -0.13646
409B -> 438B 0.17100
410B -> 437B 0.33392
410B -> 440B 0.12359
411B -> 438B -0.10774
411B -> 439B 0.12000
413B -> 437B 0.14569
413B -> 440B 0.11072
414B -> 437B 0.12883
417B -> 440B -0.16051
418B -> 440B 0.10013
419B -> 440B -0.11360

Excited State 197: 1.000-A 2.5274 eV 490.57 nm f=0.0062 <S**2>=0.000
405A -> 437A -0.11552
406A -> 437A 0.14091
409A -> 437A 0.13783
411A -> 439A 0.13202
412A -> 437A 0.29002
412A -> 439A 0.12421
413A -> 439A -0.17795
414A -> 437A 0.13124
415A -> 438A 0.34160
415A -> 440A -0.15019
417A -> 437A -0.13033
417A -> 439A 0.10783
405B -> 437B -0.11552
406B -> 437B 0.14091
409B -> 437B 0.13783

411B -> 439B 0.13202
412B -> 437B 0.29002
412B -> 439B 0.12421
413B -> 439B -0.17795
414B -> 437B 0.13124
415B -> 438B 0.34160
415B -> 440B -0.15019
417B -> 437B -0.13033
417B -> 439B 0.10783

Excited State 198: 3.000-A 2.5292 eV 490.21 nm f=0.0000 <S**2>=2.000
391A -> 438A -0.10922
391A -> 439A 0.14061
391A -> 440A -0.14289
410A -> 437A 0.12977
410A -> 438A -0.31005
410A -> 439A 0.11455
410A -> 440A 0.14118
413A -> 437A 0.19470
413A -> 439A 0.14580
416A -> 437A 0.12544
416A -> 439A 0.11782
419A -> 439A -0.13469
391B -> 438B 0.10922
391B -> 439B -0.14061
391B -> 440B 0.14289
410B -> 437B -0.12977
410B -> 438B 0.31005
410B -> 439B -0.11455
410B -> 440B -0.14118
413B -> 437B -0.19470
413B -> 439B -0.14580
416B -> 437B -0.12544
416B -> 439B -0.11782
419B -> 439B 0.13469

Excited State 199: 3.000-A 2.5309 eV 489.88 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 411A -> 438A | -0.11200 |
| 412A -> 437A | -0.38241 |
| 412A -> 439A | -0.15736 |
| 415A -> 438A | -0.39588 |
| 415A -> 440A | 0.16638 |
| 411B -> 438B | 0.11200 |
| 412B -> 437B | 0.38241 |
| 412B -> 439B | 0.15736 |
| 415B -> 438B | 0.39588 |
| 415B -> 440B | -0.16638 |

Excited State 200: 3.000-A 2.5337 eV 489.35 nm f=0.0000 <S**2>=2.000

| | |
|---|---|
| 391A -> 438A | -0.10501 |
| 391A -> 439A | 0.14755 |
| 391A -> 440A | -0.14638 |
| 410A -> 438A | 0.15967 |
| 411A -> 437A | -0.19914 |
| 411A -> 438A | -0.10128 |
| 411A -> 439A | 0.10026 |
| 412A -> 438A | -0.13229 |
| 413A -> 439A | -0.13617 |
| 414A -> 437A | -0.25316 |
| 414A -> 438A | 0.14802 |
| 414A -> 440A | 0.13076 |
| 415A -> 440A | 0.10584 |
| 416A -> 437A | -0.16017 |
| 417A -> 440A | -0.12146 |
| 391B -> 438B | 0.10501 |
| 391B -> 439B | -0.14755 |
| 391B -> 440B | 0.14638 |
| 410B -> 438B | -0.15967 |
| 411B -> 437B | 0.19914 |
| 411B -> 438B | 0.10128 |
| 411B -> 439B | -0.10026 |
| 412B -> 438B | 0.13229 |

| | |
|---|---|
| 413B -> 439B | 0.13617 |
| 414B -> 437B | 0.25316 |
| 414B -> 438B | -0.14802 |
| 414B -> 440B | -0.13076 |
| 415B -> 440B | -0.10584 |
| 416B -> 437B | 0.16017 |
| 417B -> 440B | 0.12146 |

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