Supplementary Information for

“Photogeneration of Quinone Methide from Adamantylphenol in an Ultrafast Non-adiabatic Dehydration Reaction”

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1. Deconvolution of rise time in transient absorption data

1.1 Results of transient absorption using THG of 120 fs at 800 nm as a pump pulse

Since the results of transient absorption measurements didn't show significant dynamics in first few picoseconds after excitation with 267 nm, 120 fs pulses we performed fitting of several kinetic profiles (at 425, 500 and 600 nm) focusing on first 10 ps. For the model function we used two exponential functions convoluted with identical Gaussian function to account for instrument response function (IRF) of our transient absorption spectrometer. Time constant of the first exponential function (t1) having negative amplitude then represented deconvoluted rise time of kinetic profile at that particular wavelength. In order to reduce number of free parameters, time constant for the exponential decay was fixed at 1 ns. Where needed, we expanded this model to account for coherent artifacts that could not be removed from the data without significantly affecting measured kinetic profiles. Hence, we included in the model function additional Gaussian in Figure S1 to account for two-photon absorption (TPA) signal around zero delay time, and two Gaussians were added to account for cross phase modulation signal (XPM) superimposed on exponential rise (Figures S7 to S10). It is known that, it the case of broadband chirped probe pulse, XPM signal splits in two, where the transient optical density will exhibit a gain (ΔOD<0) followed by a loss (ΔOD>0), i.e., a dispersion shape for the first XPM signal, while at increased delay times second XPM-induced pump-probe signal is present, which is out of phase with the first one. In addition, loss and gain amplitudes in this case are not identical, and only the overall signal averages to zero. This prompted us to use two Gaussian functions with the position of the center of the peak and peak amplitude being free parameters for modelling XPM artifacts.

General model:

\[ f(t) = A_1 e^{-\frac{(t - p - \sigma^2/2t_1)}{t_1}} \left(1 + \text{erf}\left(\frac{t - p - \frac{1}{2\sigma}}{\sqrt{2}\sigma}\right)\right) + A_2 e^{-\frac{(t - p - \frac{1}{2\cdot10^6})}{10^6}} \left(1 + \text{erf}\left(\frac{t - p - \frac{1}{10^6}}{\sqrt{2\sigma}}\right)\right) + A_3 e^{-\frac{t^2}{2\sigma^2}} \]

Coefficients (with 95% confidence bounds):

A1 = -0.0003891 (-0.004005, 0.003227)  A2 = 0.0003032 (0.0003006, 0.0003058)  A3 = 0.0006108 (0.0004117, 0.0008099)  p = 175.3 (-2646, 2997)  sigma = 365.9 (334.5, 397.4)  t1 = 227.9 (-84.93, 540.6)

Goodness of fit:

SSE: 6.133e-08  R-square: 0.9942  Adjusted R-square: 0.994  RMSE: 2.071e-05
Figure S1

General model:

\[ f(t) = A_1 e^{-\left(t - p - \frac{\sigma^2}{2t_1}\right)} \left[ 1 + \text{erf} \left( \frac{t - p - \sigma^2}{\sqrt{2}\sigma} \right) \right] + A_2 e^{-\left(t - p - \frac{1}{10^6}\right) \left[ 1 + \text{erf} \left( \frac{t - p - \frac{1}{10^6}}{\sqrt{2}\sigma} \right) \right]} + A_3 e^{-\left(t - p - \frac{\sigma^2}{2t_1}\right)} \]

Coefficients (with 95% confidence bounds):

- \( A_1 = -0.0003054 \) (-0.01061, 0.01)
- \( A_2 = 0.000407 \) (0.0004037, 0.0004102)
- \( p = -7.86 \) (-5054, 5038)
- \( \sigma = 555.8 \) (159.8, 951.9)
- \( t_1 = 211.4 \) (-358, 780.7)

Goodness of fit:

- SSE: 8.264e-08
- R-square: 0.9958
- Adjusted R-square: 0.9957
- RMSE: 2.396e-05
Figure S2

General model:

\[ f(t) = A_1 e^{-\left(\frac{t-p-\frac{\sigma^2}{2\tau_1}}{\tau_1}\right)} \frac{1 + erf\left(\frac{t-p-\frac{1}{\sqrt{2}\sigma}}{\sqrt{2}\sigma}\right)}{1 + erf\left(\frac{t-p-\frac{1}{10^6}}{\sqrt{2}\sigma}\right)} + A_2 e^{-\left(\frac{t-p-\frac{\sigma^2}{2\cdot10^6}}{10^6}\right)} \frac{1 + erf\left(\frac{t-p-\frac{1}{10^6}}{\sqrt{2}\sigma}\right)}{1 + erf\left(\frac{t-p-\frac{1}{10^6}}{\sqrt{2}\sigma}\right)} + A_3 e^{-\left(\frac{t-p-\frac{\sigma^2}{2\tau_1}}{\tau_1}\right)} \]

Coefficients (with 95% confidence bounds):

\[
\begin{align*}
A_1 &= -0.0004303 \quad (-0.01574, 0.01488) \\
A_2 &= 0.000353 \quad (0.000349, 0.000357) \\
p &= -86.56 \quad (-1.016e+04, 9986) \\
sigma &= 553.4 \quad (-699.3, 1806) \\
t_1 &= 248 \quad (-409.5, 905.5)
\end{align*}
\]

Goodness of fit:

SSE: 6.651e-08 R-square: 0.9954 Adjusted R-square: 0.9953 RMSE: 2.18e-05

Figure S3
To evaluate slow decay of signal at longer wavelengths that we believe originates from solvated electrons we performed simple bi-exponential fitting for the entire range of time delay points (up to 1.1 ns) for kinetic profiles corresponding to 500, 550 and 600 nm.

General model:
\[ f(t) = A_1 e^{b \cdot t} + A_2 e^{c \cdot t} \]

Coefficients (with 95% confidence bounds):
- \( A_1 = 0.001542 \) (0.00149, 0.001593)
- \( b = -2.866e-05 \) (-3.18e-05, -2.553e-05) – 35 ps
- \( A_2 = 0.002615 \) (0.002577, 0.002654)
- \( c = -6.328e-07 \) (-6.584e-07, -6.071e-07) – 1.5 ns

Goodness of fit:
- SSE: 1.287e-05
- R-square: 0.975
- Adjusted R-square: 0.9749
- RMSE: 0.000139

Figure S4

General model:
\[ f(t) = A_1 e^{b \cdot t} + A_2 e^{c \cdot t} \]

Coefficients (with 95% confidence bounds):
- \( A_1 = 0.001125 \) (0.001071, 0.00118)
- \( b = -2.801e-05 \) (-3.247e-05, -2.355e-05) – 35 ps
- \( A_2 = 0.002108 \) (0.002067, 0.002149)
- \( c = -5.481e-07 \) (-5.809e-07, -5.153e-07) – 1.8 ns

Goodness of fit:
- SSE: 1.511e-05
- R-square: 0.9471
- Adjusted R-square: 0.9469
- RMSE: 0.0001504
General model:
\[ f(t) = A_1 e^{bt} + A_2 e^{ct} \]

Coefficients (with 95% confidence bounds):
\[
\begin{align*}
A_1 &= 0.001514 \quad (0.001479, 0.001549) \\
b &= -3.506e-05 \quad (-3.748e-05, -3.264e-05) \quad – 28.5 \text{ ps} \\
A_2 &= 0.002624 \quad (0.002599, 0.002648) \\
c &= -6.594e-07 \quad (-6.764e-07, -6.425e-07) \quad – 1.5 \text{ ns}
\end{align*}
\]

Goodness of fit:
SSE: 6.179e-06  R-square: 0.9884  Adjusted R-square: 0.9883  RMSE: 9.505e-05
1.2 Results of transient absorption using sub-20-fs UV NOPA pump pulse

The same fitting procedure was used for extracting deconvoluted rise time of second set of measurements with better IRF due to the sub-20-fs UV pump pulse driving the photochemical reaction.

General model:

\[
f(t) = A_1 e^{-\frac{(t-p-\sigma^2/2t_1)^2}{t_1}} \left[1 + \text{erf} \left(\frac{t-p-\sigma^2/2t_1}{\sqrt{2}\sigma} \right) \right] + A_2 e^{-\frac{(t-p-1/10^6\sigma^2)^2}{10^6}} \left[1 + \text{erf} \left(\frac{t-p-\sigma^2/2\cdot10^6}{\sqrt{2}\sigma} \right) \right] + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}}
\]

Coefficients (with 95% confidence bounds):

| A1      | -0.001039 (-3.707, 3.705) | A2      | 0.001039 (0.0007483, 0.001329) |
|---------|--------------------------|---------|---------------------------------|
| A3      | 0.001602 (0.0007051, 0.002499) | A4      | -0.0007747 (-0.0009405, -0.000609) |
| n       | -47.11 (-50.94, -43.28)   | p       | -7.918 (-2.797e+05, 2.797e+05)  |
| r       | -4.96 (-7.359, -2.562)    | \sigma | 21.59 (17.11, 26.07)            |
| t1      | 78.4 (70.48, 86.33)       |         |                                 |

Goodness of fit:

SSE: 7.801e-07   R-square: 0.9954   Adjusted R-square: 0.9953   RMSE: 5.689e-05

Figure S7

General model:

\[
f(t) = A_1 e^{-\frac{(t-p-\sigma^2/2t_1)^2}{t_1}} \left[1 + \text{erf} \left(\frac{t-p-\sigma^2/2t_1}{\sqrt{2}\sigma} \right) \right] + A_2 e^{-\frac{(t-p-1/10^6\sigma^2)^2}{10^6}} \left[1 + \text{erf} \left(\frac{t-p-\sigma^2/2\cdot10^6}{\sqrt{2}\sigma} \right) \right] + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}}
\]
Coefficients (with 95% confidence bounds):

\[ A1 = -0.0009393 \text{ (}-0.05372, 0.05184\text{)} \quad A2 = 0.000975 \text{ (}0.0009683, 0.0009818\text{)} \]
\[ A3 = -0.01123 \text{ (}-316.9, 316.9\text{)} \quad A4 = 0.01201 \text{ (}316.9, 316.9\text{)} \]
\[ n = -13.97 \text{ (}-2.436\text{e}+04, 2.436\text{e}+04\text{)} \quad p = 19.84 \text{ (}-4415, 4455\text{)} \]
\[ r = -15.79 \text{ (}-2.547\text{e}+04, 2.547\text{e}+04\text{)} \quad \sigma = 26.4 \text{ (}544.6, 597.4\text{)} \]
\[ t1 = 82.4 \text{ (}68.44, 96.35\text{)} \]

Goodness of fit:

\[ \text{SSE: } 1.273\text{e}-06 \quad \text{R-square: } 0.9914 \quad \text{Adjusted R-square: } 0.9911 \quad \text{RMSE: } 7.267\text{e}-05 \]

Figure S8

General model:

\[ f(t) = A_1 e^{-\frac{(t-p)^2}{2t_1}} + \text{erf}\left(\frac{t-p-\frac{1}{t_1}}{\sqrt{2}\sigma}\right) + A_2 e^{-\frac{(t-p)^2}{10^6}} + \text{erf}\left(\frac{t-p-\frac{1}{10^6}}{\sqrt{2}\sigma}\right) + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}} \]

Coefficients (with 95% confidence bounds):

\[ A1 = -0.0003732 \text{ (}-0.0004635, -0.000283\text{)} \quad A2 = 0.0008317 \text{ (}0.000826, 0.0008375\text{)} \]
\[ A3 = -0.000227 \text{ (}-0.0003128, -0.0001413\text{)} \quad A4 = 0.0007324 \text{ (}0.0006103, 0.0008544\text{)} \]
\[ n = 4.683 \text{ (}1.515, 7.851\text{)} \quad p = 39.37 \text{ (}31.42, 47.33\text{)} \]
\[ r = -45.3 \text{ (}-54.89, -35.72\text{)} \quad \sigma = 21.36 \text{ (}17.14, 25.59\text{)} \]
\[ t1 = 125.4 \text{ (}98.21, 152.6\text{)} \]

Goodness of fit:

\[ \text{SSE: } 1.23\text{e}-06 \quad \text{R-square: } 0.9705 \quad \text{Adjusted R-square: } 0.9693 \quad \text{RMSE: } 7.727\text{e}-05 \]
Finally, in order to reduce the noise in kinetic profiles we integrated the signal in 400-500 nm wavelength range. By doing so we also obtained better contrast for coherent artifacts. The XPM superimposed on the initial rise of the time trace was accounted for by two Gaussian functions of opposite sign. It is reasonable to assume that TPA, being stronger at shorter wavelengths, also contributes to this artifact additionally changing the shape and ratio between positive and negative amplitudes of XPM. For negative delay times we also observe a weaker replica of the XPM artifact visible at time zero, shifted in time due to dispersion of the first cuvette window.

General model:

\[
f(t) = A_1 e^{-\left(\frac{t-p}{\sigma_1^2}\right)} + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(1 + \text{erf}\left(\frac{t-p}{\sigma_1^2}\right)\right) dt
\]

Coefficients (with 95% confidence bounds):

| Parameter | Value     | Confidence Bounds             |
|-----------|-----------|-------------------------------|
| A1        | -118.2    | (-140.1, -96.41)             |
| A2        | 199.8     | (199.1, 200.6)               |
| A3        | -108.7    | (-133, -84.33)               |
| A4        | 314.7     | (298.4, 331)                 |
| n         | -2.628    | (-4.677, -0.5791)            |
| p         | 28.17     | (18.37, 37.98)               |
| r         | -43.34    | (-49.82, -36.86)             |
| \(\sigma\) | 23.98     | (20.97, 26.98)               |
| t1        | 110       | (98.23, 121.8)               |

Goodness of fit:

SSE: 2.085e+04   R-square: 0.9966   Adjusted R-square: 0.9965   RMSE: 9.302
Figure S10

2. Intensity dependence of transient absorption spectra

In order to clarify the origin of the signal at longer wavelengths that we attributed to solvated electrons we measured excitation intensity dependence on the transient absorption spectra for both the sample and pure solvent at fixed delay of 10 ps that show quadratic dependence in the case of pure solvent as expected for two-photon ionization. Intensity dependence for sample is almost linear suggesting that it stems from free electrons resulting from radical cation formation which is one photon process as is shown in Figure 8. with only minor contribution of two-photon ionization of solvent molecules.

Figure S11  Excitation intensity dependence on the transient absorption spectra of adamantylphenol at fixed delay of 10 ps at 425 nm (left) and 600 nm (right) that show linear dependence.
Figure S12 Excitation intensity dependence on the transient absorption spectra in pure solvent at fixed delay of 10 ps at 425 nm (left) and 600 nm (right) that show quadratic dependence as expected for two-photon ionization.

3. Absorption spectra and transient absorption spectra

Figure S13 Absorption spectrum of 3 in CH$_3$CN-H$_2$O (1:1) (for the path of 1 mm), at concentration $c = 5.0 \times 10^{-3}$ M that was used for fs-TA experiment with 280 nm sub-20-fs pump pulses from SHG of NOPA.
Figure S14 fs-TA data using sub-20-fs UV NOPA pump pulse and WLC driven by the SH of Ti:sapphire together with spectral and kinetic profiles for the selected wavelengths. Only strong ground state bleach is observed below 285nm.
4. Laser flash photolysis measurements

Figure S15 Nanosecond decay of transient absorption at 400 nm for Ar-purged (left) and O₂-purged (right) CH₃CN-H₂O (1:1 v/v) solution of 3 (2.0 × 10⁻⁴ M). The energy of the laser pulse at 266 nm was set to 17 mJ/pulse. The bottom panels correspond to the weighted residuals between the measured value and the calculated according to the single exponential decay model.
Figure S16 Millisecond decay of transient absorption at 400 nm for Ar-purged (left) and O$_2$-purged (right) CH$_3$CN-H$_2$O (1:1 v/v) solution of 3 ($2.0 \times 10^{-4}$ M). The energy of the laser pulse at 266 nm was set to 17 mJ/pulse. The bottom panels correspond to the weighted residuals between the measured value and the calculated according to the single exponential decay model.
Figure S17 Decay of transient absorption at 420 nm for Ar-purged (left) and O$_2$-purged CH$_3$CN-H$_2$O (1:1 v/v) solution of 3 (2.0 × 10$^{-4}$ M). The energy of the laser pulse at 266 nm was set to 17 mJ/pulse. The bottom panels correspond to the weighted residuals between the measured value and the calculated according to the single exponential decay model.

5. Fluorescence upconversion measurements

5.1 Instrument response function

Instrument response function measurement was taken with identical experimental conditions prior to FLUC measurements of adamantylphenol.
5.2 Global analysis of FIUC data

The spectro-temporal signal can be described by three components: the first describes a rise of the signal in 0.46 ps, the second describe a decay of ca, 1/3 of the total signal. The last component is set to 2 ns (infinity in our spanned time window). The presence of the first component is necessary because the rise of the signal is much slower than the measured IRF (630 fs). If we carry out the global fit procedure with free IRF we can remove the 0.5 ps component but the IRF would be 1.2 ps (and the time zero would be accordingly shifted). It is noteworthy that the first component equalizes the sum of the other two components. This speaks for a signal, which is delayed by 0.5 ps and is not directly populated upon excitation.
Since FIUC measurements could not be performed at magic angle, it is possible to ascribe 22 ps decay to rotational anisotropy decay. Actually, 22 ps is too short for such processes (typically 100-200 ps in conventional solvents) but due to the limited scan range of 50 ps we cannot distinguish between 20 ps and 100 ps. In global analysis, the effect to change the time constant would be only to change the relative amplitude of the second and third DAS component (see Figure S19). To check this explanation, we carried out an analysis where we changed the second component in order to obtain a ratio 2:1 between the second and the third component. Indeed, a pure rotational anisotropy would induce a reduction by 2/3 of the initial signal with respect to the fully randomized one. The outcome of this analysis is shown in Figure S20. Under the 2:1 condition, the second time constant changed to 90 ps, which is compatible with a rotational diffusion process.
In order to verify both IRF and the presence of the 0.5 ps rise in the adamantylphenol signal we performed additional FLUC measurements using anisole as a reference system. Only the two long components were necessary for the fitting of data. Any attempts to add a rise component or to impose 1 ps IRF were rejected by the fitting. When the IRF parameter was set free the fitting procedure gives 0.79±0.08 ps.

**5.3 FLUC of anisole molecule**

*Figure S20.* Results of global analysis with imposed rotational anisotropy decay.

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*S18*
Figure S21. Fluorescence intensity kinetics of anisole in acetonitrile used as a reference molecule. IRF is represented by KB parameter.

6. Time-correlated single photon counting (TC-SPC) measurements

Figure S22. Normalized excitation and emission spectra of 3 in CH$_3$CN-H$_2$O (1:1).
Figure S23. Decay of fluorescence of 3 in CH$_3$CN-H$_2$O (1:1) at 310 nm ($\lambda_{\text{exc}} = 280$ nm).

Figure S24. Time-resolved emission spectra ($\lambda_{\text{em}} = 280$ nm) of 3 in CH$_3$CN-H$_2$O (1:1).
7. Computations

a) [UV-VIS Spectrum Image]

b) [UV-VIS Spectrum Image]
Figure S25. Simulated spectra of $3(S_0)$ (a), $3'(S_0)$ (b) and $4(S_0)$ (c) computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

Table S1. Vertical excitation of singlet $3(S_0)$, $3'(S_0)$ and $4(S_0)$ computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

| Excited State | 1: Singlet-A | 5.1087 eV 242.69 nm f=0.0686 $<S^2>=0.000$ |
|---------------|--------------|---------------------------------------------|
| 65 -> 72      | 0.18262      |                                             |
| 65 -> 73      | -0.15138     |                                             |
| 66 -> 67      | 0.16718      |                                             |
| 66 -> 68      | 0.51394      |                                             |
| 66 -> 69      | -0.20974     |                                             |
| 66 -> 70      | 0.10196      |                                             |
| 66 -> 71      | -0.18071     |                                             |
| 66 -> 72      | 0.12491      |                                             |

| Excited State | 2: Singlet-A | 5.7839 eV 214.36 nm f=0.0363 $<S^2>=0.000$ |
|---------------|--------------|---------------------------------------------|
| 65 -> 68      | -0.283477    |                                             |
| 65 -> 69      | 0.11648      |                                             |
| 65 -> 71      | 0.10547      |                                             |
| 66 -> 67      | -0.12447     |                                             |
| 66 -> 68      | -0.11290     |                                             |
| 66 -> 70      | 0.22629      |                                             |
| 66 -> 72      | 0.40683      |                                             |
| 66 -> 73      | -0.28317     |                                             |
| 66 -> 74      | -0.10558     |                                             |
| 66 -> 75      | -0.12508     |                                             |

| Excited State | 3: Singlet-A | 6.1077 eV 203.00 nm f=0.0025 $<S^2>=0.000$ |
|---------------|--------------|---------------------------------------------|
| 66 -> 67      | 0.44139      |                                             |
| 66 -> 68      | -0.21640     |                                             |
| 66 -> 69      | -0.32170     |                                             |
| 66 -> 71      | 0.15996      |                                             |
| 66 -> 73      | -0.15506     |                                             |
66 -> 79  0.10660
66 -> 80  -0.15515
66 -> 87  0.12105

Excited State 4:  Singlet-A  6.5006 eV  190.73 nm  f=0.6735  <S**2>=0.000
  65 -> 67  0.20094
  65 -> 68  0.38317
  65 -> 69  -0.18439
  65 -> 71  -0.14889
  65 -> 72  -0.17980
  65 -> 73  0.14288
  66 -> 68  0.16577
  66 -> 72  0.22198
  66 -> 73  -0.20566

Excited State 5:  Singlet-A  6.5834 eV  188.33 nm  f=0.2238  <S**2>=0.000
  65 -> 68  0.29816
  65 -> 70  0.22921
  65 -> 72  0.29211
  65 -> 73  -0.17491
  66 -> 68  -0.28954
  66 -> 69  -0.10111
  66 -> 70  0.15612
  66 -> 71  -0.12467
  66 -> 72  0.18275

Excited State 6:  Singlet-A  6.6599 eV  186.17 nm  f=0.1924  <S**2>=0.000
  65 -> 70  0.17454
  65 -> 72  0.24766
  65 -> 73  -0.16263
  66 -> 69  0.18771
  66 -> 70  -0.20373
  66 -> 71  0.33314
  66 -> 73  -0.25941
  66 -> 74  0.10692
  66 -> 77  0.11473

Excited State 7:  Singlet-A  6.7638 eV  183.31 nm  f=0.0199  <S**2>=0.000
  65 -> 67  -0.24540
  65 -> 68  0.17010
  65 -> 69  0.17996
  66 -> 69  -0.11654
  66 -> 70  0.24439
  66 -> 71  0.30911
  66 -> 74  0.21175
  66 -> 75  0.13174
  66 -> 77  -0.15307

Excited State 8:  Singlet-A  6.8752 eV  180.33 nm  f=0.0132  <S**2>=0.000
  65 -> 67  0.34962
  65 -> 68  -0.14467
  65 -> 69  -0.26185
  65 -> 80  -0.12008
  66 -> 70  0.27748
  66 -> 71  0.20187
  66 -> 77  -0.24350
Excited State 9: Singlet-A 6.9561 eV 178.24 nm f=0.0039 \( <S^2> = 0.000 \)

| Transition | Energy Difference |
|------------|-------------------|
| 65 -> 67   | -0.11889          |
| 65 -> 68   | 0.12482           |
| 66 -> 67   | 0.14771           |
| 66 -> 69   | 0.31207           |
| 66 -> 70   | 0.18337           |
| 66 -> 71   | -0.14322          |
| 66 -> 72   | -0.20247          |
| 66 -> 73   | -0.18267          |
| 66 -> 74   | -0.23626          |
| 66 -> 77   | -0.23886          |
| 66 -> 80   | -0.15244          |

Excited State 10: Singlet-A 7.0514 eV 175.83 nm f=0.1781 \( <S^2> = 0.000 \)

| Transition | Energy Difference |
|------------|-------------------|
| 61 -> 67   | 0.13613           |
| 61 -> 68   | 0.28181           |
| 61 -> 69   | -0.13513          |
| 64 -> 67   | 0.22713           |
| 64 -> 68   | 0.42523           |
| 64 -> 69   | -0.18396          |
| 64 -> 71   | -0.13788          |

Excited State 11: Singlet-A 7.2542 eV 170.91 nm f=0.0037 \( <S^2> = 0.000 \)

| Transition | Energy Difference |
|------------|-------------------|
| 66 -> 67   | 0.25364           |
| 66 -> 69   | 0.10128           |
| 66 -> 74   | -0.12555          |
| 66 -> 75   | 0.27907           |
| 66 -> 76   | -0.27006          |
| 66 -> 77   | 0.10211           |
| 66 -> 78   | 0.10481           |
| 66 -> 80   | 0.30641           |
| 66 -> 85   | -0.13211          |
| 66 -> 87   | -0.13786          |
| 66 -> 91   | -0.10806          |

Excited State 12: Singlet-A 7.3271 eV 169.21 nm f=0.0214 \( <S^2> = 0.000 \)

| Transition | Energy Difference |
|------------|-------------------|
| 61 -> 70   | -0.13078          |
| 64 -> 67   | 0.16672           |
| 64 -> 68   | -0.14207          |
| 64 -> 70   | -0.11157          |
| 65 -> 67   | 0.11754           |
| 65 -> 68   | 0.10175           |
| 65 -> 69   | 0.23738           |
| 65 -> 70   | -0.23529          |
| 65 -> 73   | -0.23757          |
| 65 -> 75   | -0.10061          |
| 66 -> 74   | 0.14129           |
| 66 -> 76   | 0.13957           |
| 66 -> 79   | -0.11357          |

Excited State 13: Singlet-A 7.4212 eV 167.07 nm f=0.0204 \( <S^2> = 0.000 \)

| Transition | Energy Difference |
|------------|-------------------|
| 61 -> 72   | -0.11630          |
| 64 -> 70   | -0.13696          |
| 64 -> 72   | -0.16005          |
65 -> 68       0.13340
65 -> 71       0.26197
65 -> 74       0.12814
66 -> 71       0.15442
66 -> 73       0.16426
66 -> 74       -0.25409
66 -> 75       -0.15151
66 -> 78       0.21682
66 -> 79       0.17787

Excited State 14: Singlet-A
Energy: 7.4573 eV, Wavelength: 166.26 nm, f=0.0259, $<S^2>=0.000$
61 -> 72       0.19530
61 -> 73       -0.14194
63 -> 67       -0.13802
63 -> 68       -0.13154
64 -> 70       0.17230
64 -> 72       0.29671
64 -> 73       -0.19253
65 -> 69       0.10227
65 -> 70       -0.10079
65 -> 73       -0.15364
66 -> 73       0.10313
66 -> 74       -0.10137
66 -> 75       -0.11640
66 -> 78       0.12806

63 -> 67       0.19835
63 -> 68       0.11297
64 -> 67       -0.17400
65 -> 67       -0.10996
65 -> 68       0.12119
65 -> 70       -0.10651
65 -> 71       0.34525
65 -> 73       -0.11673
65 -> 74       0.14850
66 -> 73       -0.11564
66 -> 74       0.14847
66 -> 75       0.13261
66 -> 78       -0.15470

Excited State 17: Singlet-A
Energy: 7.5808 eV, Wavelength: 163.55 nm, f=0.0039, $<S^2>=0.000$
63 -> 68       -0.15469
65 -> 70       0.12542
65 -> 71       0.23223
| Transition | Value |
|------------|-------|
| 65 -> 73   | 0.11150 |
| 65 -> 74   | 0.13387 |
| 66 -> 67   | 0.21320 |
| 66 -> 69   | 0.14707 |
| 66 -> 72   | 0.13206 |
| 66 -> 74   | 0.11239 |
| 66 -> 76   | 0.28533 |
| 66 -> 78   | 0.12865 |
| 66 -> 79   | -0.16330 |

Excited State 18: Singlet-A 7.6011 eV 163.11 nm f=0.0029 <S**2>=0.000

| Transition | Value |
|------------|-------|
| 61 -> 67   | 0.12001 |
| 63 -> 67   | 0.23519 |
| 63 -> 69   | 0.15306 |
| 64 -> 67   | -0.15972 |
| 65 -> 67   | -0.10886 |
| 65 -> 69   | -0.13605 |
| 65 -> 70   | -0.19323 |
| 65 -> 71   | -0.18505 |
| 65 -> 72   | 0.14640 |
| 65 -> 77   | 0.20131 |
| 66 -> 76   | 0.16363 |
| 66 -> 78   | 0.13182 |

Excited State 19: Singlet-A 7.6282 eV 162.53 nm f=0.0040 <S**2>=0.000

| Transition | Value |
|------------|-------|
| 62 -> 67   | 0.39720 |
| 62 -> 68   | 0.12847 |
| 62 -> 69   | 0.10331 |
| 63 -> 67   | -0.21446 |
| 63 -> 69   | -0.16449 |
| 65 -> 69   | -0.12222 |
| 65 -> 72   | 0.18490 |
| 65 -> 73   | 0.11608 |
| 65 -> 77   | 0.12134 |
| 65 -> 80   | 0.10649 |

Excited State 20: Singlet-A 7.6470 eV 162.13 nm f=0.0092 <S**2>=0.000

| Transition | Value |
|------------|-------|
| 3'(S0)     |       |

Excited State 1: Singlet-A 5.0995 eV 243.13 nm f=0.0675 <S**2>=0.000

| Transition | Value |
|------------|-------|
| 65 -> 73   | 0.15256 |
| 65 -> 74   | 0.19317 |
| Energy Difference | Excited State | Singlet-A | Excitation Energy | Wavelength | oscillator strength | $S^2$ |
|-------------------|--------------|-----------|-------------------|-------------|--------------------|-------|
| 66 -> 67          | 2            | -0.25325  | 5.8683 eV         | 211.28 nm   | 0.0087             | 0.000 |
| 66 -> 68          |              | 0.57219   |                   |             |                    |       |
| 65 -> 67          |              | -0.19263  |                   |             |                    |       |
| 65 -> 68          |              | 0.41669   |                   |             |                    |       |
| 66 -> 67          |              | -0.10915  |                   |             |                    |       |
| 66 -> 71          |              | 0.16072   |                   |             |                    |       |
| 66 -> 72          |              | -0.20314  |                   |             |                    |       |
| 66 -> 73          |              | -0.27565  |                   |             |                    |       |
| 66 -> 74          |              | -0.31541  |                   |             |                    |       |
| 66 -> 67          | 3            | 0.43542   | 6.1549 eV         | 201.44 nm   | 0.0016             | 0.000 |
| 66 -> 68          |              | 0.20061   |                   |             |                    |       |
| 66 -> 69          |              | 0.30906   |                   |             |                    |       |
| 66 -> 70          |              | 0.19323   |                   |             |                    |       |
| 66 -> 74          |              | -0.13420  |                   |             |                    |       |
| 66 -> 78          |              | 0.12510   |                   |             |                    |       |
| 66 -> 80          |              | -0.16780  |                   |             |                    |       |
| 66 -> 67          | 4            | -0.24549  | 6.4801 eV         | 191.33 nm   | 0.6394             | 0.000 |
| 65 -> 68          |              | 0.41119   |                   |             |                    |       |
| 65 -> 74          |              | -0.11444  |                   |             |                    |       |
| 66 -> 72          |              | 0.16839   |                   |             |                    |       |
| 66 -> 73          |              | 0.24171   |                   |             |                    |       |
| 66 -> 74          |              | 0.28727   |                   |             |                    |       |
| 66 -> 75          |              | -0.11811  |                   |             |                    |       |
| 66 -> 68          | 5            | -0.13360  | 6.5857 eV         | 188.26 nm   | 0.1956             | 0.000 |
| 65 -> 68          |              | -0.20975  |                   |             |                    |       |
| 65 -> 71          |              | 0.19997   |                   |             |                    |       |
| 65 -> 72          |              | -0.17328  |                   |             |                    |       |
| 65 -> 73          |              | -0.20600  |                   |             |                    |       |
| 65 -> 74          |              | -0.20426  |                   |             |                    |       |
| 66 -> 68          |              | 0.21143   |                   |             |                    |       |
| 66 -> 69          |              | 0.27955   |                   |             |                    |       |
| 66 -> 70          |              | -0.18008  |                   |             |                    |       |
| 66 -> 72          |              | -0.15911  |                   |             |                    |       |
| 66 -> 68          | 6            | -0.21562  | 6.6969 eV         | 185.14 nm   | 0.2546             | 0.000 |
| 65 -> 73          |              | -0.21331  |                   |             |                    |       |
| 65 -> 74          |              | 0.10707   |                   |             |                    |       |
| 66 -> 69          |              | -0.27985  |                   |             |                    |       |
| Reaction   | Energy  |
|------------|---------|
| 65 -> 67   | 0.33259 |
| 65 -> 68   | 0.19870 |
| 65 -> 69   | 0.29945 |
| 65 -> 70   | -0.19803|
| 65 -> 71   | 0.12017 |
| 65 -> 72   | -0.14156|
| 65 -> 73   | 0.11899 |
| 65 -> 74   | -0.17858|
| 65 -> 75   | -0.15733|
| 65 -> 76   | 0.12946 |
| 65 -> 77   | -0.25705|
| 65 -> 78   | -0.11232|

**Excited State 7:** Singlet-A  6.7772 eV  182.94 nm  f=0.0783  <S**2>=0.000

| Reaction   | Energy  |
|------------|---------|
| 66 -> 70   | 0.32346 |
| 66 -> 71   | -0.23824|
| 66 -> 72   | 0.33259 |
| 66 -> 73   | -0.29945|
| 66 -> 74   | -0.19803|
| 66 -> 75   | 0.12017 |
| 66 -> 76   | -0.14156|
| 66 -> 77   | 0.11899 |
| 66 -> 78   | -0.15733|
| 66 -> 79   | 0.12946 |
| 66 -> 80   | -0.25705|
| 66 -> 81   | -0.11232|

**Excited State 8:** Singlet-A  6.9186 eV  179.20 nm  f=0.0100  <S**2>=0.000

| Reaction   | Energy  |
|------------|---------|
| 67 -> 68   | 0.18919 |
| 67 -> 69   | 0.17178 |
| 68 -> 69   | 0.17018 |
| 68 -> 70   | 0.42500 |
| 68 -> 71   | -0.13662|
| 68 -> 72   | 0.18313 |
| 68 -> 73   | -0.11608|
| 68 -> 74   | 0.12946 |
| 68 -> 75   | -0.25705|
| 68 -> 76   | -0.11232|

**Excited State 9:** Singlet-A  7.0260 eV  176.46 nm  f=0.0658  <S**2>=0.000

| Reaction   | Energy  |
|------------|---------|
| 61 -> 62   | 0.14314 |
| 61 -> 63   | 0.16102 |
| 62 -> 63   | 0.11650 |
| 62 -> 64   | -0.13885|
| 63 -> 64   | -0.21718|
| 63 -> 65   | 0.25631 |
| 64 -> 65   | 0.10259 |
| 64 -> 66   | -0.15235|
| 64 -> 67   | -0.18836|
| 64 -> 68   | 0.18379 |
| 65 -> 66   | -0.18836|
| 65 -> 67   | 0.18379 |
| 65 -> 68   | -0.16181|
| 66 -> 67   | -0.14700|
| 66 -> 68   | -0.11670|
| 66 -> 69   | -0.10231|

**Excited State 10:** Singlet-A  7.0320 eV  176.31 nm  f=0.0750  <S**2>=0.000

| Reaction   | Energy  |
|------------|---------|
| 61 -> 62   | 0.17920 |
| 61 -> 63   | -0.14882|
| 62 -> 63   | -0.20441|
| Transition | Energy  |
|------------|---------|
| 64 -> 68   | 0.25637 |
| 66 -> 69   | 0.20776 |
| 66 -> 70   | 0.20345 |
| 66 -> 72   | -0.23590|
| 66 -> 73   | 0.12123 |
| 66 -> 77   | 0.18222 |
| 66 -> 80   | 0.10465 |

**Excited State 11:** Singlet-A 7.2366 eV 171.33 nm f=0.0133 <S**2>=0.000

| Transition | Energy  |
|------------|---------|
| 55 -> 68   | -0.15961|
| 60 -> 67   | -0.11513|
| 60 -> 68   | 0.24107 |
| 61 -> 67   | 0.11821 |
| 61 -> 68   | -0.16330|
| 63 -> 67   | -0.20257|
| 63 -> 68   | 0.25887 |
| 64 -> 67   | -0.18815|
| 64 -> 68   | 0.33184 |
| 66 -> 75   | 0.11665 |

**Excited State 12:** Singlet-A 7.2514 eV 170.98 nm f=0.0092 <S**2>=0.000

| Transition | Energy  |
|------------|---------|
| 64 -> 68   | -0.20236|
| 65 -> 69   | 0.22270 |
| 65 -> 71   | 0.14561 |
| 65 -> 72   | -0.13443|
| 65 -> 74   | 0.12322 |
| 66 -> 67   | -0.14993|
| 66 -> 68   | -0.11292|
| 66 -> 73   | 0.15888 |
| 66 -> 75   | 0.26415 |
| 66 -> 80   | -0.21744|

**Excited State 13:** Singlet-A 7.2601 eV 170.77 nm f=0.0232 <S**2>=0.000

| Transition | Energy  |
|------------|---------|
| 60 -> 68   | -0.10687|
| 61 -> 68   | 0.16187 |
| 63 -> 68   | -0.19973|
| 64 -> 67   | 0.10825 |
| 65 -> 69   | -0.15887|
| 65 -> 71   | -0.15147|
| 65 -> 72   | 0.10331 |
| 65 -> 74   | -0.11254|
| 66 -> 67   | -0.11265|
| 66 -> 73   | 0.16742 |
| 66 -> 75   | 0.31529 |
| 66 -> 80   | -0.21649|

**Excited State 14:** Singlet-A 7.4108 eV 167.30 nm f=0.0098 <S**2>=0.000

| Transition | Energy  |
|------------|---------|
| 65 -> 69   | -0.12106|
| Transition | Change | | Transition | Change | | Transition | Change |
|------------|--------|---|------------|--------|---|------------|--------|
| 65 -> 70   | 0.47320|   | 66 -> 70   | 0.14386|   | 66 -> 74   | 0.28301|
| 65 -> 73   | 0.17172|   | 66 -> 74   | -0.11268|   | 66 -> 76   | 0.14252|
| 65 -> 74   | -0.17618| | 66 -> 79   | 0.11319|   | 66 -> 79   | 0.26173|
| Excited State 15: Singlet-A 7.5333 eV 164.58 nm f=0.0031 <S**2>=0.000 | | | Excited State 16: Singlet-A 7.5719 eV 163.74 nm f=0.0068 <S**2>=0.000 | | | Excited State 17: Singlet-A 7.5772 eV 163.63 nm f=0.0092 <S**2>=0.000 | |
| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 66 -> 74 | 0.10169    |        |        |    |       |
| 66 -> 76 | -0.12977   |        |        |    |       |
| 61 -> 71 | 0.10592    |        |        |    |       |
| 63 -> 67 | 0.46116    |        |        |    |       |
| 63 -> 68 | 0.17404    |        |        |    |       |
| 63 -> 69 | -0.20926   |        |        |    |       |
| 64 -> 67 | 0.10499    |        |        |    |       |
| 65 -> 72 | 0.14774    |        |        |    |       |
| 66 -> 75 | -0.12665   |        |        |    |       |
| Excited State 18: Singlet-A | 7.6276 eV 162.55 nm | f=0.0131 <S^2>=0.000 |

| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 61 -> 71 | 0.10592    |        |        |    |       |
| 63 -> 67 | 0.46116    |        |        |    |       |
| 63 -> 68 | 0.17404    |        |        |    |       |
| 63 -> 69 | -0.20926   |        |        |    |       |
| 64 -> 67 | 0.10499    |        |        |    |       |
| 65 -> 72 | 0.14774    |        |        |    |       |
| 66 -> 75 | -0.12665   |        |        |    |       |
| Excited State 19: Singlet-A | 7.6772 eV 161.50 nm | f=0.0009 <S^2>=0.000 |

| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 61 -> 67 | 0.31727    |        |        |    |       |
| 62 -> 67 | 0.10158    |        |        |    |       |
| 62 -> 69 | -0.12550   |        |        |    |       |
| 63 -> 67 | -0.11758   |        |        |    |       |
| 64 -> 67 | 0.11730    |        |        |    |       |
| 65 -> 72 | 0.14499    |        |        |    |       |
| 66 -> 75 | -0.23226   |        |        |    |       |
| 66 -> 78 | 0.24790    |        |        |    |       |
| Excited State 20: Singlet-A | 7.7080 eV 160.85 nm | f=0.0139 <S^2>=0.000 |

| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 57 -> 62 | -0.10971   |        |        |    |       |
| 60 -> 62 | 0.66874    |        |        |    |       |
| 60 -> 69 | -0.10595   |        |        |    |       |
| 61 -> 62 | -0.10442   |        |        |    |       |
| Excited State 1: Singlet-A | 3.2613 eV 380.17 nm | f=0.0020 <S^2>=0.000 |

| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 57 -> 62 | -0.10971   |        |        |    |       |
| 60 -> 62 | 0.66874    |        |        |    |       |
| 60 -> 69 | -0.10595   |        |        |    |       |
| 61 -> 62 | -0.10442   |        |        |    |       |
| Excited State 2: Singlet-A | 3.3676 eV 368.17 nm | f=0.2359 <S^2>=0.000 |

| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 56 -> 62 | 0.15489    |        |        |    |       |
| 59 -> 62 | 0.66611    |        |        |    |       |
| Excited State 3: Singlet-A | 4.8271 eV 256.85 nm | f=0.3394 <S^2>=0.000 |

| State   | Transition | E (eV) | λ (nm) | f  | <S^2> |
|---------|------------|--------|--------|----|-------|
| 56 -> 62 | 0.15489    |        |        |    |       |
| 59 -> 62 | 0.66611    |        |        |    |       |
| Excited State 4: Singlet-A | 5.2575 eV 235.82 nm | f=0.0224 <S^2>=0.000 |
| Transition | Energy | Wavelength | Oscillator Strength | Dipole Moment | Quadratic Overlap |
|------------|--------|-------------|---------------------|--------------|-------------------|
| 55 -> 62   | 0.24020|             |                     |              |                   |
| 57 -> 62   | 0.32750|             |                     |              |                   |
| 58 -> 62   | 0.53123|             |                     |              |                   |
| Excited State 5: Singlet-A | 5.4225 eV | 228.65 nm | 0.0206 | 0.000 |
| 51 -> 62   | -0.12394|             |                     |              |                   |
| 57 -> 62   | 0.51068 |             |                     |              |                   |
| 58 -> 62   | -0.38197|             |                     |              |                   |
| 60 -> 62   | 0.12934 |             |                     |              |                   |
| 60 -> 75   | 0.11319 |             |                     |              |                   |
| Excited State 6: Singlet-A | 5.8104 eV | 213.38 nm | 0.0811 | 0.000 |
| 60 -> 69   | -0.10156|             |                     |              |                   |
| 61 -> 65   | 0.11988 |             |                     |              |                   |
| 61 -> 66   | -0.16479|             |                     |              |                   |
| 61 -> 69   | 0.52261 |             |                     |              |                   |
| 61 -> 70   | -0.25378|             |                     |              |                   |
| 61 -> 71   | -0.15760|             |                     |              |                   |
| 61 -> 72   | 0.15804 |             |                     |              |                   |
| Excited State 7: Singlet-A | 5.9596 eV | 208.04 nm | 0.0014 | 0.000 |
| 61 -> 63   | 0.48527 |             |                     |              |                   |
| 61 -> 64   | -0.36774|             |                     |              |                   |
| 61 -> 67   | 0.12908 |             |                     |              |                   |
| 61 -> 69   | -0.12808|             |                     |              |                   |
| 61 -> 76   | 0.52261 |             |                     |              |                   |
| 61 -> 83   | -0.13561|             |                     |              |                   |
| Excited State 8: Singlet-A | 5.9707 eV | 207.65 nm | 0.0021 | 0.000 |
| 50 -> 62   | -0.10411|             |                     |              |                   |
| 56 -> 62   | 0.61023 |             |                     |              |                   |
| 59 -> 62   | -0.14914|             |                     |              |                   |
| 60 -> 69   | 0.12243 |             |                     |              |                   |
| 61 -> 75   | 0.16080 |             |                     |              |                   |
| Excited State 9: Singlet-A | 6.0694 eV | 204.28 nm | 0.0059 | 0.000 |
| 50 -> 62   | -0.18077|             |                     |              |                   |
| 56 -> 62   | -0.15554|             |                     |              |                   |
| 57 -> 62   | -0.15774|             |                     |              |                   |
| 60 -> 62   | 0.10106 |             |                     |              |                   |
| 60 -> 66   | -0.11297|             |                     |              |                   |
| 60 -> 69   | 0.44769 |             |                     |              |                   |
| 60 -> 70   | -0.19398|             |                     |              |                   |
| 60 -> 71   | -0.15360|             |                     |              |                   |
| 60 -> 72   | 0.15213 |             |                     |              |                   |
| 61 -> 69   | 0.12146 |             |                     |              |                   |
| Excited State 10: Singlet-A | 6.3117 eV | 196.44 nm | 0.0898 | 0.000 |
| 48 -> 62   | 0.14601 |             |                     |              |                   |
| 52 -> 62   | -0.19078|             |                     |              |                   |
| 55 -> 62   | 0.37015 |             |                     |              |                   |
| 56 -> 62   | 0.11571 |             |                     |              |                   |
| 57 -> 62   | -0.13399|             |                     |              |                   |
| 58 -> 62   | -0.11187|             |                     |              |                   |
| 60 -> 69   | -0.11986|             |                     |              |                   |
| 61 -> 75   | -0.34282|             |                     |              |                   |
| 61 -> 76   | 0.10433 |             |                     |              |                   |
| Excited State | Singlet-A | E (eV) | λ (nm) | f | \( <S^2> \) |
|--------------|-----------|-------|-------|---|-------------|
| 11:          | 6.3361    | 195.68| 0.1254| 0.000|            |
| 48 -> 62     | 0.12844   |       |       |     |             |
| 52 -> 62     | 0.19441   |       |       |     |             |
| 55 -> 62     | 0.42813   |       |       |     |             |
| 56 -> 62     | -0.15968  |       |       |     |             |
| 57 -> 62     | -0.10203  |       |       |     |             |
| 58 -> 62     | -0.13537  |       |       |     |             |
| 61 -> 65     | -0.11486  |       |       |     |             |
| 61 -> 75     | 0.31378   |       |       |     |             |
| 12:          | 6.5464    | 189.39| 0.0168| 0.000|            |
| 52 -> 62     | 0.11912   |       |       |     |             |
| 53 -> 62     | -0.34185  |       |       |     |             |
| 61 -> 64     | 0.11707   |       |       |     |             |
| 61 -> 65     | 0.42694   |       |       |     |             |
| 61 -> 66     | 0.15668   |       |       |     |             |
| 61 -> 68     | -0.24281  |       |       |     |             |
| 13:          | 6.5664    | 188.82| 0.0210| 0.000|            |
| 52 -> 62     | 0.12283   |       |       |     |             |
| 53 -> 62     | 0.54445   |       |       |     |             |
| 54 -> 62     | -0.15483  |       |       |     |             |
| 61 -> 65     | 0.27291   |       |       |     |             |
| 61 -> 66     | 0.10059   |       |       |     |             |
| 61 -> 68     | -0.13274  |       |       |     |             |
| 14:          | 6.6321    | 186.95| 0.0059| 0.000|            |
| 52 -> 62     | 0.21588   |       |       |     |             |
| 59 -> 63     | -0.10968  |       |       |     |             |
| 61 -> 63     | 0.18125   |       |       |     |             |
| 61 -> 64     | 0.39381   |       |       |     |             |
| 61 -> 65     | -0.18252  |       |       |     |             |
| 61 -> 67     | 0.35056   |       |       |     |             |
| 61 -> 76     | -0.13161  |       |       |     |             |
| 15:          | 6.7175    | 184.57| 0.1327| 0.000|            |
| 48 -> 62     | 0.12530   |       |       |     |             |
| 49 -> 62     | -0.10176  |       |       |     |             |
| 50 -> 62     | 0.49735   |       |       |     |             |
| 51 -> 62     | 0.15506   |       |       |     |             |
| 52 -> 62     | 0.24300   |       |       |     |             |
| 60 -> 63     | 0.10024   |       |       |     |             |
| 60 -> 65     | 0.10055   |       |       |     |             |
| 60 -> 69     | 0.13337   |       |       |     |             |
| 61 -> 75     | -0.12867  |       |       |     |             |
| 16:          | 6.7323    | 184.16| 0.0240| 0.000|            |
| 50 -> 62     | -0.11276  |       |       |     |             |
| 60 -> 63     | 0.38374   |       |       |     |             |
| 60 -> 64     | -0.12947  |       |       |     |             |
| 60 -> 65     | 0.29853   |       |       |     |             |
| 60 -> 66     | 0.13797   |       |       |     |             |
| 60 -> 67     | 0.20315   |       |       |     |             |
| 60 -> 68     | -0.18130  |       |       |     |             |
| 60 -> 74     | 0.15167   |       |       |     |             |
| 60 -> 75     | -0.11365  |       |       |     |             |
| Transition | Energy | Wavelength | Intensity | Spin Quantum | Multiplicity |
|------------|--------|-------------|-----------|--------------|--------------|
| 60 -> 82   | 0.10826|             |           |              |              |

**Excited State 17:** Singlet-A

| Transition | Energy | Wavelength | Intensity | Spin Quantum | Multiplicity |
|------------|--------|-------------|-----------|--------------|--------------|
| 51 -> 62  | 0.19809|             |           |              |              |
| 52 -> 62  | -0.13778|            |           |              |              |
| 61 -> 65  | 0.12179 |             |           |              |              |
| 61 -> 66  | -0.32045|            |           |              |              |
| 61 -> 71  | 0.37277 |             |           |              |              |
| 61 -> 72  | -0.10643|            |           |              |              |
| 61 -> 75  | 0.18705 |             |           |              |              |
| 61 -> 82  | -0.14416|            |           |              |              |

**Excited State 18:** Singlet-A

| Transition | Energy | Wavelength | Intensity | Spin Quantum | Multiplicity |
|------------|--------|-------------|-----------|--------------|--------------|
| 51 -> 62  | 0.23961 |             |           |              |              |
| 52 -> 62  | -0.30597|            |           |              |              |
| 53 -> 62  | 0.11174 |             |           |              |              |
| 54 -> 62  | 0.33444 |             |           |              |              |
| 61 -> 66  | 0.22523 |             |           |              |              |
| 61 -> 71  | -0.21236|            |           |              |              |
| 61 -> 72  | 0.10585 |             |           |              |              |
| 61 -> 75  | 0.12622 |             |           |              |              |

**Excited State 19:** Singlet-A

| Transition | Energy | Wavelength | Intensity | Spin Quantum | Multiplicity |
|------------|--------|-------------|-----------|--------------|--------------|
| 50 -> 62  | -0.10572|            |           |              |              |
| 51 -> 62  | -0.16944|            |           |              |              |
| 52 -> 62  | 0.20051 |             |           |              |              |
| 53 -> 62  | 0.15656 |             |           |              |              |
| 54 -> 62  | 0.56134 |             |           |              |              |
| 61 -> 75  | -0.10428|            |           |              |              |

**Excited State 20:** Singlet-A

| Transition | Energy | Wavelength | Intensity | Spin Quantum | Multiplicity |
|------------|--------|-------------|-----------|--------------|--------------|
| 48 -> 62  | 0.11683 |             |           |              |              |
| 50 -> 62  | -0.29686|            |           |              |              |
| 51 -> 62  | 0.33407 |             |           |              |              |
| 52 -> 62  | 0.25193 |             |           |              |              |
| 57 -> 62  | 0.14211 |             |           |              |              |
| 60 -> 75  | -0.26983|            |           |              |              |
| 60 -> 76  | 0.10816 |             |           |              |              |
| 61 -> 75  | -0.11101|            |           |              |              |
Figure S26. Simulated spectra of $3(S_1)$ (a), $3'(S_1)$ (b) and $4(S_1)$ (c) computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

Table S2. Vertical excitation of singlet $3(S_1)$, $3'(S_1)$ and $4(S_1)$ computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

| Excited State | Singlet- A | $E_{exc}$ (eV) | $\lambda$ (nm) | $f$ | $<S^2>$ |
|---------------|------------|----------------|----------------|-----|---------|
| 1: $3(S_1)$   | 4.3469     | 285.23         | 0.0998         | 0.000 |
| 65 -> 67      | -0.11363   |                |                |      |
| 65 -> 73      | 0.10934    |                |                |      |
| 66 -> 67      | 0.65474    |                |                |      |
| 2: $3'(S_1)$  | 5.2463     | 236.33         | 0.0264         | 0.000 |
| 65 -> 67      | 0.46561    |                |                |      |
| 66 -> 67      | 0.16994    |                |                |      |
| 66 -> 70      | -0.17408   |                |                |      |
| 66 -> 72      | -0.20237   |                |                |      |
| 66 -> 73      | -0.31205   |                |                |      |
| 66 -> 74      | -0.15276   |                |                |      |
| 66 -> 75      | 0.15631    |                |                |      |
| 3: $4(S_1)$   | 5.7634     | 215.12         | 0.0048         | 0.000 |
| 66 -> 68      | 0.47585    |                |                |      |
| 66 -> 69      | -0.37595   |                |                |      |
| 66 -> 71      | -0.14595   |                |                |      |
| 66 -> 80      | -0.15398   |                |                |      |
| 66 -> 87      | -0.12117   |                |                |      |
| 4: $4(S_1)$   | 5.8863     | 210.63         | 0.4484         | 0.000 |
| 65 -> 67      | 0.46580    |                |                |      |
| 66 -> 70      | 0.16736    |                |                |      |
| 66 -> 72      | 0.18975    |                |                |      |
| 66 -> 73      | 0.34171    |                |                |      |
| 66 -> 74      | 0.13735    |                |                |      |
| 66 -> 75      | -0.14492   |                |                |      |
66 -> 77 -0.12596

Excited State 5:  Singlet-A  6.2675 eV  197.82 nm  f=0.0426  <S**2>=0.000

65 -> 70  0.12932
65 -> 72  0.12555
65 -> 73  0.19766
66 -> 67  -0.12152
66 -> 69  -0.20436
66 -> 71  0.41057
66 -> 72  0.18798
66 -> 73  -0.17547
66 -> 74  0.15208

Excited State 6:  Singlet-A  6.4080 eV  193.48 nm  f=0.0561  <S**2>=0.000

61 -> 67  0.14385
64 -> 67  -0.20472
65 -> 68  -0.14395
65 -> 69  0.11143
65 -> 70  0.11491
65 -> 72  0.12360
65 -> 73  0.15590
65 -> 74  0.11443
66 -> 68  -0.12157
66 -> 70  0.32943
66 -> 71  -0.24352
66 -> 74  -0.26581
66 -> 77  0.11834

Excited State 7:  Singlet-A  6.4175 eV  193.20 nm  f=0.1377  <S**2>=0.000

64 -> 67  0.14356
65 -> 70  -0.14660
65 -> 72  -0.15875
65 -> 73  -0.26765
65 -> 74  -0.10182
65 -> 75  0.12752
66 -> 69  -0.11631
66 -> 70  0.36989
66 -> 71  0.10414
66 -> 72  0.10341
66 -> 77  0.24330
66 -> 84  0.12723

Excited State 8:  Singlet-A  6.5970 eV  187.94 nm  f=0.1235  <S**2>=0.000

61 -> 67  -0.12471
64 -> 67  0.17092
65 -> 70  0.12128
65 -> 72  0.11821
65 -> 73  0.17285
66 -> 68  0.14016
66 -> 69  0.30049
66 -> 70  0.15689
66 -> 72  -0.28251
66 -> 76  0.10776
66 -> 77  0.21842
66 -> 80  -0.15287

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Excited State 9: Singlet-A  6.6004 eV  187.84 nm  f=0.1897  <S**2>=0.000

Excited State 10: Singlet-A  6.7710 eV  183.11 nm  f=0.0207  <S**2>=0.000

Excited State 11: Singlet-A  6.9437 eV  178.56 nm  f=0.0086  <S**2>=0.000

Excited State 12: Singlet-A  7.0235 eV  176.53 nm  f=0.0140  <S**2>=0.000

Excited State 13: Singlet-A  7.0472 eV  175.93 nm  f=0.0450  <S**2>=0.000

Excited State 14: Singlet-A  7.1004 eV  174.62 nm  f=0.0057  <S**2>=0.000
| Transition | Energy Difference |
|------------|------------------|
| 66 -> 71   | -0.15415         |
| 66 -> 72   | 0.17782          |
| 66 -> 73   | -0.13888         |
| 66 -> 75   | -0.13660         |
| 66 -> 76   | 0.31129          |
| 66 -> 78   | 0.22880          |
| 66 -> 79   | -0.12806         |
| 66 -> 87   | 0.14480          |

Excited State 15: Singlet-A 7.2155 eV 171.83 nm f=0.0017 <S**2>=0.000
| Transition | Energy Difference |
|------------|------------------|
| 66 -> 71   | -0.20008         |
| 66 -> 74   | 0.22419          |
| 66 -> 75   | 0.38263          |
| 66 -> 76   | 0.19638          |
| 66 -> 78   | 0.16542          |
| 66 -> 79   | 0.12165          |
| 66 -> 81   | 0.24879          |

Excited State 16: Singlet-A 7.3037 eV 169.75 nm f=0.0169 <S**2>=0.000
| Transition | Energy Difference |
|------------|------------------|
| 65 -> 69   | -0.16215         |
| 65 -> 70   | 0.30400          |
| 65 -> 71   | 0.15029          |
| 65 -> 72   | 0.17054          |
| 65 -> 73   | -0.17442         |
| 65 -> 77   | 0.17437          |
| 66 -> 68   | 0.20215          |
| 66 -> 69   | 0.13135          |
| 66 -> 72   | 0.13251          |
| 66 -> 74   | -0.13651         |
| 66 -> 79   | -0.13793         |

Excited State 17: Singlet-A 7.3705 eV 168.22 nm f=0.0193 <S**2>=0.000
| Transition | Energy Difference |
|------------|------------------|
| 62 -> 67   | 0.11427          |
| 65 -> 70   | -0.22265         |
| 65 -> 71   | 0.42409          |
| 65 -> 74   | 0.27313          |
| 66 -> 74   | 0.11382          |

Excited State 18: Singlet-A 7.3923 eV 167.72 nm f=0.0112 <S**2>=0.000
| Transition | Energy Difference |
|------------|------------------|
| 64 -> 68   | -0.12555         |
| 65 -> 68   | -0.13176         |
| 65 -> 69   | -0.15819         |
| 65 -> 71   | -0.10978         |
| 66 -> 68   | -0.13009         |
| 66 -> 69   | -0.20535         |
| 66 -> 70   | -0.20280         |
| 66 -> 73   | 0.17696          |
| 66 -> 75   | -0.14423         |
| 66 -> 77   | 0.17420          |
| 66 -> 84   | 0.26785          |
| 66 -> 87   | 0.16371          |
| 66 -> 89   | 0.13925          |

Excited State 19: Singlet-A 7.4310 eV 166.85 nm f=0.0042 <S**2>=0.000
| Transition | Energy Difference |
|------------|------------------|
| 62 -> 67   | 0.55922          |
| 63 -> 67   | -0.30032         |
| Excited State | 20: Singlet-A | 7.4654 eV | 166.08 nm | f=0.0253 | <S**2>=0.000 |
|--------------|---------------|------------|-----------|---------|--------------|
| 57 -> 67     | -0.15761      | 0.25564    |           |         |              |
| 60 -> 67     | -0.17293      |           |           |         |              |
| 61 -> 67     |               | 0.12236    |           |         |              |
| 63 -> 67     | 0.20288       |           |           |         |              |
| 63 -> 68     | 0.10298       |           |           |         |              |
| 64 -> 67     | 0.16226       |           |           |         |              |
| 64 -> 70     | 0.12340       |           |           |         |              |
| 64 -> 72     | 0.13218       |           |           |         |              |
| 64 -> 73     | 0.12650       |           |           |         |              |
| 65 -> 69     | 0.17793       |           |           |         |              |
| 65 -> 71     | -0.12829      |           |           |         |              |
| 65 -> 72     | -0.15242      |           |           |         |              |
| 65 -> 73     | 0.10293       |           |           |         |              |

| 3'(S₁)       |
|--------------|---------------|------------|-----------|---------|--------------|
| Excited State 1: Singlet-A | 3.7412 eV | 331.40 nm | f=0.0819 | <S**2>=0.000 |
| 65 -> 67     | 0.11014       |           |           |         |              |
| 66 -> 67     | 0.68106       |           |           |         |              |

| Excited State 2: Singlet-A | 4.6040 eV | 269.30 nm | f=0.0321 | <S**2>=0.000 |
| 65 -> 67     | 0.56725       |           |           |         |              |
| 66 -> 67     | -0.13870      |           |           |         |              |
| 66 -> 70     | 0.15196       |           |           |         |              |
| 66 -> 72     | -0.28243      |           |           |         |              |
| 66 -> 73     | 0.12449       |           |           |         |              |

| Excited State 3: Singlet-A | 5.3692 eV | 230.92 nm | f=0.2437 | <S**2>=0.000 |
| 65 -> 67     | 0.37328       |           |           |         |              |
| 66 -> 70     | -0.25080      |           |           |         |              |
| 66 -> 71     | 0.14030       |           |           |         |              |
| 66 -> 72     | 0.43911       |           |           |         |              |
| 66 -> 73     | -0.16359      |           |           |         |              |

| Excited State 4: Singlet-A | 5.6775 eV | 218.38 nm | f=0.0393 | <S**2>=0.000 |
| 66 -> 68     | 0.48051       |           |           |         |              |
| 66 -> 69     | 0.21811       |           |           |         |              |
| 66 -> 71     | 0.27541       |           |           |         |              |
| 66 -> 72     | -0.12093      |           |           |         |              |
| 66 -> 73     | 0.11966       |           |           |         |              |
| 66 -> 77     | 0.17748       |           |           |         |              |
| 66 -> 80     | 0.10231       |           |           |         |              |
| 66 -> 88     | 0.10301       |           |           |         |              |

| Excited State 5: Singlet-A | 5.8059 eV | 213.55 nm | f=0.0125 | <S**2>=0.000 |
| 61 -> 67     | 0.21109       |           |           |         |              |
| 64 -> 67     | 0.63802       |           |           |         |              |

| Excited State 6: Singlet-A | 6.0982 eV | 203.31 nm | f=0.0321 | <S**2>=0.000 |
| 60 -> 67     | -0.13307      |           |           |         |              |
| 63 -> 67     | 0.18506       |           |           |         |              |
| Transition | Energy Difference |
|------------|-------------------|
| 65 -> 70   | -0.12143          |
| 65 -> 72   | 0.20124           |
| 65 -> 73   | -0.10246          |
| 66 -> 68   | 0.15706           |
| 66 -> 69   | 0.36070           |
| 66 -> 71   | -0.26549          |
| 66 -> 72   | 0.20124           |
| 66 -> 73   | -0.10246          |
| 66 -> 74   | -0.12278          |
| 66 -> 75   | 0.10893           |
| 66 -> 77   | -0.10484          |

**Excited State 7: Singlet-A**
- Energy: 6.1670 eV
- Wavelength: 201.04 nm
- Oscillator Strength: 0.0358
- <S^2>: 0.000

| Transition | Energy Difference |
|------------|-------------------|
| 60 -> 67   | -0.26696          |
| 61 -> 67   | -0.16186          |
| 62 -> 67   | -0.15570          |
| 63 -> 67   | 0.42936           |
| 65 -> 70   | 0.12385           |
| 65 -> 71   | 0.11257           |
| 66 -> 69   | -0.19055          |
| 66 -> 71   | 0.22150           |

**Excited State 8: Singlet-A**
- Energy: 6.2994 eV
- Wavelength: 196.82 nm
- Oscillator Strength: 0.0401
- <S^2>: 0.000

| Transition | Energy Difference |
|------------|-------------------|
| 65 -> 70   | 0.12385           |
| 65 -> 71   | -0.24075          |
| 65 -> 73   | 0.10344           |
| 66 -> 70   | 0.49776           |
| 66 -> 71   | 0.10848           |
| 66 -> 73   | -0.19579          |
| 66 -> 75   | -0.12318          |

**Excited State 9: Singlet-A**
- Energy: 6.3456 eV
- Wavelength: 195.39 nm
- Oscillator Strength: 0.2732
- <S^2>: 0.000

| Transition | Energy Difference |
|------------|-------------------|
| 65 -> 70   | 0.13797           |
| 65 -> 71   | 0.36066           |
| 65 -> 73   | -0.15484          |
| 66 -> 70   | 0.16028           |
| 66 -> 71   | 0.20755           |
| 66 -> 72   | 0.12480           |
| 66 -> 73   | -0.11107          |

**Excited State 10: Singlet-A**
- Energy: 6.5740 eV
- Wavelength: 188.60 nm
- Oscillator Strength: 0.0201
- <S^2>: 0.000

| Transition | Energy Difference |
|------------|-------------------|
| 66 -> 68   | 0.30228           |
| 66 -> 69   | -0.27865          |
| 66 -> 70   | 0.10359           |
| 66 -> 71   | -0.19299          |
| 66 -> 72   | 0.12831           |
| 66 -> 73   | 0.24538           |
Excited State 11: Singlet-A  6.6881 eV  185.38 nm  f=0.0064  <S**2>=0.000
  62 -> 67  0.14607
  65 -> 68  0.40685
  65 -> 69  0.24738
  65 -> 71  0.13061
  65 -> 72  -0.10338
  65 -> 77  0.10362
  66 -> 70  -0.11575
  66 -> 71  -0.10106
  66 -> 73  0.16537
  66 -> 74  -0.14119
  66 -> 75  -0.15116

Excited State 12: Singlet-A  6.7483 eV  183.73 nm  f=0.0042  <S**2>=0.000
  63 -> 67  0.62910
  66 -> 67  0.17944

Excited State 13: Singlet-A  6.8130 eV  181.98 nm  f=0.0282  <S**2>=0.000
  61 -> 67  -0.10012
  63 -> 67  -0.12369
  65 -> 68  0.12509
  65 -> 69  0.12284
  65 -> 70  0.12369
  66 -> 68  0.12233
  66 -> 69  -0.13626
  66 -> 74  0.34329
  66 -> 75  0.19682
  66 -> 76  0.25206
  66 -> 77  -0.18646
  66 -> 79  -0.17092

Excited State 14: Singlet-A  6.8574 eV  180.80 nm  f=0.0109  <S**2>=0.000
  55 -> 67  -0.11540
  60 -> 67  0.17397
  61 -> 67  0.46889
  63 -> 67  0.32212
  64 -> 67  -0.11274
  65 -> 68  0.13605
  65 -> 69  0.13693

Excited State 15: Singlet-A  6.9119 eV  179.38 nm  f=0.0011  <S**2>=0.000
  65 -> 68  -0.13985
  65 -> 69  -0.19176
  66 -> 73  0.20453
| Transition   | E   |
|--------------|-----|
| 66 -> 74     | 0.10833 |
| 66 -> 75     | -0.21682 |
| 66 -> 76     | 0.40416 |
| 66 -> 77     | 0.11735 |
| 66 -> 78     | 0.17223 |

Excited State 16: Singlet-A  6.9305 eV  178.90 nm  f=0.0004  <S**2>=0.000

| Transition   | E   |
|--------------|-----|
| 66 -> 71     | -0.16976 |
| 66 -> 72     | 0.18127 |
| 66 -> 73     | 0.10820 |
| 66 -> 74     | 0.14913 |
| 66 -> 75     | 0.27533 |
| 66 -> 76     | -0.17369 |
| 66 -> 77     | 0.11647 |
| 66 -> 80     | 0.29154 |
| 66 -> 82     | -0.13630 |
| 66 -> 84     | 0.14874 |
| 66 -> 86     | -0.22583 |

Excited State 17: Singlet-A  7.0404 eV  176.10 nm  f=0.0045  <S**2>=0.000

| Transition   | E   |
|--------------|-----|
| 54 -> 67     | -0.27715 |
| 55 -> 67     | -0.11471 |
| 57 -> 67     | 0.31587 |
| 58 -> 67     | -0.13712 |
| 60 -> 67     | 0.27667 |
| 61 -> 67     | -0.30157 |
| 63 -> 67     | 0.11875 |
| 64 -> 67     | 0.19074 |

Excited State 18: Singlet-A  7.1215 eV  174.10 nm  f=0.0161  <S**2>=0.000

| Transition   | E   |
|--------------|-----|
| 65 -> 71     | 0.21683 |
| 65 -> 77     | 0.10122 |
| 66 -> 70     | -0.13827 |
| 66 -> 71     | -0.21970 |
| 66 -> 73     | -0.21152 |
| 66 -> 74     | 0.26985 |
| 66 -> 75     | -0.20493 |
| 66 -> 76     | -0.17266 |
| 66 -> 81     | 0.20995 |
| 66 -> 90     | -0.13606 |

Excited State 19: Singlet-A  7.1697 eV  172.93 nm  f=0.0264  <S**2>=0.000

| Transition   | E   |
|--------------|-----|
| 64 -> 68     | 0.10086 |
| 65 -> 69     | 0.17893 |
| 65 -> 70     | 0.28654 |
| 65 -> 71     | -0.15964 |
| 65 -> 73     | -0.23539 |
| 65 -> 77     | -0.13935 |

| Transition   | E   |
|--------------|-----|
| 66 -> 84     | 0.14874 |
| 66 -> 86     | -0.22583 |
| 66 -> 74     | 0.17223 |
| 66 -> 75     | 0.11647 |
| 66 -> 77     | 0.11647 |
| 66 -> 80     | 0.29154 |
| 66 -> 82     | -0.13630 |
| 66 -> 84     | 0.14874 |
| 66 -> 86     | -0.22583 |
|   | 66 -> 68 | -0.13585 |
|---|---------|----------|
|   | 66 -> 69 | 0.13084 |
|   | 66 -> 72 | 0.12834 |
|   | 66 -> 75 | -0.20559 |
|   | 66 -> 81 | 0.10804 |
| Excited State 20: | Singlet-A | 7.2095 eV, 171.97 nm, f=0.0042, $<S^2>=0.000$ |
|   | 64 -> 68 | -0.13806 |
|   | 65 -> 69 | -0.13252 |
|   | 66 -> 68 | 0.14455 |
|   | 66 -> 69 | -0.18201 |
|   | 66 -> 73 | 0.28508 |
|   | 66 -> 74 | 0.19676 |
|   | 66 -> 75 | 0.13469 |
|   | 66 -> 76 | -0.14642 |
|   | 66 -> 77 | 0.12400 |
|   | 66 -> 83 | 0.14642 |
|   | 66 -> 84 | 0.21489 |
|   | 66 -> 86 | 0.11057 |
|   | 66 -> 88 | -0.12447 |

| 4($S_1$) |
|---|---|
| Excited State 1: | Singlet-A, 2.3459 eV, 528.52 nm, f=0.1661, $<S^2>=0.000$ |
|   | 60 -> 62 | -0.18621 |
|   | 61 -> 62 | 0.68148 |
| Excited State 2: | Singlet-A, 2.8766 eV, 431.00 nm, f=0.0361, $<S^2>=0.000$ |
|   | 60 -> 62 | 0.66908 |
|   | 61 -> 62 | 0.19065 |
| Excited State 3: | Singlet-A, 4.0877 eV, 303.31 nm, f=0.2274, $<S^2>=0.000$ |
|   | 59 -> 62 | 0.68505 |
| Excited State 4: | Singlet-A, 4.7746 eV, 259.67 nm, f=0.0189, $<S^2>=0.000$ |
|   | 51 -> 62 | 0.14423 |
|   | 58 -> 62 | 0.67036 |
| Excited State 5: | Singlet-A, 4.8437 eV, 255.97 nm, f=0.0408, $<S^2>=0.000$ |
|   | 52 -> 62 | 0.13798 |
|   | 56 -> 62 | -0.41228 |
|   | 57 -> 62 | 0.49752 |
| Excited State 6: | Singlet-A, 5.1966 eV, 238.59 nm, f=0.0160, $<S^2>=0.000$ |
|   | 57 -> 62 | -0.14340 |
|   | 61 -> 66 | 0.27143 |
|   | 61 -> 69 | 0.57178 |
|   | 61 -> 72 | -0.15498 |
| Excited State 7: | Singlet-A, 5.3029 eV, 233.80 nm, f=0.0189, $<S^2>=0.000$ |
|   | 56 -> 62 | 0.52475 |
|   | 57 -> 62 | 0.39313 |
|   | 61 -> 69 | 0.14111 |
| Excited State 8: | Singlet-A, 5.4339 eV, 228.17 nm, f=0.0003, $<S^2>=0.000$ |
|   | 61 -> 63 | 0.47905 |
|   | 61 -> 64 | 0.36519 |
|   | 61 -> 65 | 0.14576 |
| Transition | Energy Difference | 
|------------|------------------|
| 61 -> 67   | 0.14216          |
| 61 -> 76   | 0.13001          |
| 61 -> 83   | 0.17026          |
| **Excited State 9:** Singlet-A | 5.5804 eV 222.18 nm f=0.1500 $<S^2>=0.000$ |
| 55 -> 62   | -0.31583         |
| 56 -> 62   | -0.12602         |
| 61 -> 70   | -0.14320         |
| 61 -> 72   | 0.22840          |
| 61 -> 73   | 0.47730          |
| 50 -> 62   | -0.15939         |
| 51 -> 62   | 0.23323          |
| 52 -> 62   | 0.17753          |
| 53 -> 62   | -0.12804         |
| 54 -> 62   | -0.14978         |
| 57 -> 62   | -0.11632         |
| 60 -> 66   | 0.14800          |
| 60 -> 69   | 0.39545          |
| 60 -> 70   | -0.11521         |
| 60 -> 73   | 0.26464          |
| **Excited State 10:** Singlet-A | 5.7708 eV 214.85 nm f=0.0035 $<S^2>=0.000$ |
| 50 -> 62   | -0.15939         |
| 51 -> 62   | 0.23323          |
| 52 -> 62   | 0.17753          |
| 53 -> 62   | -0.12804         |
| 54 -> 62   | -0.14978         |
| 57 -> 62   | -0.11632         |
| 60 -> 66   | 0.14800          |
| 60 -> 69   | 0.39545          |
| 60 -> 70   | -0.11521         |
| 60 -> 73   | 0.26464          |
| **Excited State 11:** Singlet-A | 5.9045 eV 209.98 nm f=0.0173 $<S^2>=0.000$ |
| 53 -> 62   | 0.35652          |
| 54 -> 62   | 0.50182          |
| 55 -> 62   | -0.18985         |
| 60 -> 69   | 0.16870          |
| 60 -> 73   | 0.10076          |
| **Excited State 12:** Singlet-A | 6.0113 eV 206.25 nm f=0.0061 $<S^2>=0.000$ |
| 52 -> 62   | -0.20073         |
| 61 -> 64   | -0.24083         |
| 61 -> 65   | 0.44618          |
| 61 -> 66   | 0.18417          |
| 61 -> 67   | 0.13141          |
| 61 -> 68   | -0.27645         |
| **Excited State 13:** Singlet-A | 6.0123 eV 206.22 nm f=0.0276 $<S^2>=0.000$ |
| 50 -> 62   | -0.10822         |
| 52 -> 62   | 0.55875          |
| 57 -> 62   | -0.10837         |
| 60 -> 69   | -0.20184         |
| 61 -> 65   | 0.16749          |
| 61 -> 68   | -0.10806         |
| **Excited State 14:** Singlet-A | 6.1127 eV 202.83 nm f=0.2500 $<S^2>=0.000$ |
| 54 -> 62   | 0.16439          |
| 55 -> 62   | 0.44749          |
| 61 -> 63   | 0.11166          |
| 61 -> 64   | -0.21586         |
| 61 -> 65   | -0.13353         |
| 61 -> 67   | 0.23774          |
| 61 -> 68   | 0.11114          |
| 61 -> 72   | 0.18228          |
| 61 -> 73   | 0.13056          |
| **Excited State 15:** Singlet-A | 6.1382 eV 201.99 nm f=0.1912 $<S^2>=0.000$ |
| Transition | Energy |
|------------|--------|
| 51 -> 62   | -0.22118 |
| 52 -> 62   | 0.10061 |
| 55 -> 62   | 0.28296 |
| 61 -> 63   | -0.14966 |
| 61 -> 64   | 0.27928 |
| 61 -> 65   | 0.16527 |
| 61 -> 67   | -0.26724 |
| 61 -> 70   | -0.12944 |
| 61 -> 73   | 0.17849 |
| 61 -> 76   | -0.10539 |

Excited State 16: Singlet-A
- Energy: 6.1486 eV
- Wavelength: 201.65 nm
- Oscillator Strength: 0.0051
- Extinction Coefficient: 0.000

| Transition | Energy |
|------------|--------|
| 48 -> 62   | -0.11183 |
| 51 -> 62   | 0.52817 |
| 54 -> 62   | 0.10506 |
| 58 -> 62   | -0.11743 |
| 60 -> 69   | -0.18880 |
| 61 -> 64   | 0.14988 |
| 61 -> 67   | -0.15403 |

Excited State 17: Singlet-A
- Energy: 6.2347 eV
- Wavelength: 198.86 nm
- Oscillator Strength: 0.0033
- Extinction Coefficient: 0.000

| Transition | Energy |
|------------|--------|
| 53 -> 62   | 0.57193 |
| 54 -> 62   | -0.38602 |

Excited State 18: Singlet-A
- Energy: 6.2767 eV
- Wavelength: 197.53 nm
- Oscillator Strength: 0.0319
- Extinction Coefficient: 0.000

| Transition | Energy |
|------------|--------|
| 61 -> 65   | -0.10372 |
| 61 -> 66   | 0.41365 |
| 61 -> 69   | -0.10218 |
| 61 -> 71   | 0.17161 |
| 61 -> 72   | 0.36576 |
| 61 -> 73   | -0.20471 |
| 61 -> 80   | 0.15270 |
| 61 -> 82   | -0.10904 |

Excited State 19: Singlet-A
- Energy: 6.3842 eV
- Wavelength: 194.21 nm
- Oscillator Strength: 0.0356
- Extinction Coefficient: 0.000

| Transition | Energy |
|------------|--------|
| 60 -> 65   | 0.11075 |
| 60 -> 66   | -0.11895 |
| 60 -> 69   | -0.27219 |
| 60 -> 72   | 0.31547 |
| 60 -> 73   | 0.45674 |

Excited State 20: Singlet-A
- Energy: 6.5064 eV
- Wavelength: 190.56 nm
- Oscillator Strength: 0.0051
- Extinction Coefficient: 0.000

| Transition | Energy |
|------------|--------|
| 50 -> 62   | 0.57666 |
| 52 -> 62   | 0.10920 |
| 60 -> 63   | -0.15351 |
| 60 -> 65   | -0.14740 |
Figure S27. Simulated spectra of (a) 3rc(S₀) and (b) 3′rc(S₀) radical cation computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

Table S3. Vertical excitation of singlet 3rc(S₀) and 3′rc(S₀) radical cation computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

| Excited State | Energy (eV) | f | Ω² | λ (nm) | ¥ |
|---------------|-------------|---|-----|--------|---|
| 3rc(S₁)       |             |   |     |        |   |
| 59B → 66B     | -0.15457    |   |     |        |   |
| 61B → 66B     | 0.11944     |   |     |        |   |
| 62B → 66B     | 0.77524     |   |     |        |   |
| 63B → 66B     | 0.20536     |   |     |        |   |
| 64B → 66B     | 0.16174     |   |     |        |   |
| 65B → 66B     | -0.51803    |   |     |        |   |
Excited State 2: 2.049 Å 2.6073 eV 475.53 nm f=0.0043 <S**2>=0.800
54B -> 66B -0.16827
56B -> 66B 0.22734
61B -> 66B 0.66706
62B -> 66B 0.27386
64B -> 66B -0.20340
65B -> 66B 0.54240

Excited State 3: 2.046 Å 3.0481 eV 406.76 nm f=0.0098 <S**2>=0.796
59B -> 66B 0.35213
62B -> 66B -0.15439
63B -> 66B 0.65081
64B -> 66B 0.58119
65B -> 66B 0.12863

Excited State 4: 2.042 Å 3.3568 eV 369.35 nm f=0.0004 <S**2>=0.793
55B -> 66B 0.17292
61B -> 66B 0.17387
63B -> 66B -0.63809
64B -> 66B 0.69643

Excited State 5: 2.081 Å 3.4391 eV 360.52 nm f=0.0159 <S**2>=0.833
62A -> 68A -0.10679
66A -> 67A 0.13291
50B -> 66B -0.11636
55B -> 66B 0.39005
56B -> 66B -0.29338
59B -> 66B 0.12802
61B -> 66B 0.52952
62B -> 66B -0.32440
64B -> 66B -0.17803
65B -> 66B -0.46640

Excited State 6: 2.131 Å 3.5818 eV 346.15 nm f=0.0308 <S**2>=0.885
62A -> 68A 0.16429
63A -> 67A -0.12385
66A -> 67A -0.18677
66A -> 68A -0.10662
53B -> 66B 0.10487
55B -> 66B -0.37466
56B -> 66B 0.53430
57B -> 66B 0.16803
59B -> 66B -0.12228
61B -> 66B 0.24285
62B -> 66B -0.34918
62B -> 67B -0.11541
64B -> 66B 0.10463
65B -> 66B -0.38238

Excited State 7: 2.072 Å 3.9117 eV 316.96 nm f=0.0025 <S**2>=0.823
48B -> 66B 0.14317
49B -> 66B 0.13649
50B -> 66B 0.23466
51B -> 66B -0.14343
53B -> 66B 0.21999
54B -> 66B 0.62193
| Transition | Energy (eV) | Wavelength (nm) | f | \langle S^2 \rangle |
|------------|------------|----------------|---|-------------------|
| 56B -> 66B | 0.10362    |                |    |                   |
| 58B -> 66B | -0.16168   |                |    |                   |
| 59B -> 66B | 0.50713    |                |    |                   |
| 61B -> 66B | 0.17831    |                |    |                   |
| 62B -> 66B | 0.10544    |                |    |                   |
| 63B -> 66B | -0.21946   |                |    |                   |
| 64B -> 66B | -0.14012   |                |    |                   |
| 50B -> 66B | -0.18931   |                |    |                   |
| 53B -> 66B | -0.38536   |                |    |                   |
| 54B -> 66B | -0.17680   |                |    |                   |
| 55B -> 66B | -0.13869   |                |    |                   |
| 56B -> 66B | 0.12573    |                |    |                   |
| 57B -> 66B | -0.16561   |                |    |                   |
| 58B -> 66B | 0.57773    |                |    |                   |
| 59B -> 66B | 0.49795    |                |    |                   |
| 61B -> 66B | -0.10623   |                |    |                   |
| 62B -> 66B | 0.14692    |                |    |                   |
| 63B -> 66B | -0.17057   |                |    |                   |
| 59A -> 68A | -0.10646   |                |    |                   |
| 61A -> 68A | -0.10297   |                |    |                   |
| 62A -> 68A | 0.43649    |                |    |                   |
| 63A -> 67A | 0.20615    |                |    |                   |
| 63A -> 68A | 0.13339    |                |    |                   |
| 65A -> 68A | -0.14689   |                |    |                   |
| 66A -> 67A | 0.52827    |                |    |                   |
| 58B -> 66B | 0.40475    |                |    |                   |
| 62B -> 67B | -0.29432   |                |    |                   |
| 62B -> 68B | 0.10327    |                |    |                   |
| 65B -> 67B | 0.17668    |                |    |                   |
| 62A -> 68A | -0.19120   |                |    |                   |
| 66A -> 67A | -0.23618   |                |    |                   |
| 50B -> 66B | 0.15732    |                |    |                   |
| 53B -> 66B | 0.24720    |                |    |                   |
| 54B -> 66B | 0.37184    |                |    |                   |
| 56B -> 66B | -0.14143   |                |    |                   |
| 57B -> 66B | 0.11316    |                |    |                   |
| 58B -> 66B | 0.65050    |                |    |                   |
| 59B -> 66B | -0.30466   |                |    |                   |
| 62B -> 67B | 0.12239    |                |    |                   |
| 65B -> 66B | 0.12153    |                |    |                   |
| 60B -> 66B | 0.97732    |                |    |                   |
| 61B -> 66B | -0.11019   |                |    |                   |
| 46B -> 66B | 0.15237    |                |    |                   |
| 48B -> 66B | -0.49192   |                |    |                   |
| 49B -> 66B | -0.21740   |                |    |                   |
| 54B -> 66B | -0.10092   |                |    |                   |
57B -> 66B  0.69885
59B -> 66B  0.32923

Excited State 13: 2.099-A  5.0035 eV  247.79 nm  f=0.0057  <S**2>=0.851
66A -> 67A  0.13182
45B -> 66B  -0.12784
46B -> 66B  0.20940
47B -> 66B  0.37042
48B -> 66B  0.65446
52B -> 66B  -0.11522
53B -> 66B  0.15524
54B -> 66B  -0.13360
55B -> 66B  0.11876
56B -> 66B  0.14783
57B -> 66B  0.36188
61B -> 66B  -0.15275

Excited State 14: 2.471-A  5.1126 eV  242.51 nm  f=0.0032  <S**2>=1.276
59A -> 67A  0.11047
62A -> 67A  -0.53612
63A -> 67A  -0.21843
63A -> 68A  0.26775
65A -> 67A  0.23229
65A -> 68A  -0.14195
66A -> 68A  0.63073
46B -> 66B  -0.10668
57B -> 66B  0.11779

Excited State 15: 2.145-A  5.1379 eV  241.31 nm  f=0.0077  <S**2>=0.900
62A -> 67A  -0.19297
66A -> 68A  0.10228
42B -> 66B  -0.17897
45B -> 66B  -0.12779
46B -> 66B  0.50161
47B -> 66B  0.20705
48B -> 66B  -0.16430
49B -> 66B  -0.18811
51B -> 66B  0.10966
52B -> 66B  -0.12757
53B -> 66B  0.42344
54B -> 66B  -0.11721
55B -> 66B  -0.20756
57B -> 66B  -0.42510
59B -> 66B  0.12921

Excited State 16: 2.916-A  5.2953 eV  234.14 nm  f=0.0735  <S**2>=1.876
62A -> 67A  -0.35163
62A -> 68A  -0.29781
63A -> 68A  -0.24917
65A -> 68A  0.20239
66A -> 67A  0.46677
66A -> 68A  -0.28987
55B -> 66B  -0.19426
57B -> 66B  0.11132
62B -> 68B  -0.38066
| Transition | Value |
|------------|-------|
| 65B -> 68B | 0.23116 |
| 62A -> 67A | 0.27060 |
| 63A -> 67A | 0.25988 |
| 63A -> 68A | 0.14453 |
| 65A -> 67A | -0.20114 |
| 66A -> 67A | 0.35312 |
| 66A -> 68A | 0.40979 |
| 43B -> 66B | 0.10326 |
| 48B -> 66B | -0.14884 |
| 54B -> 66B | 0.13013 |
| 55B -> 66B | -0.32511 |
| 56B -> 66B | 0.19865 |
| 62B -> 67B | 0.35054 |
| 65B -> 67B | -0.21507 |

Excited State 17: 2.557-A  5.4042 eV  229.42 nm  f=0.1478  <S**2>=1.385

| Transition | Value |
|------------|-------|
| 66A -> 67A | 0.13507 |
| 43B -> 66B | -0.16258 |
| 48B -> 66B | -0.20047 |
| 50B -> 66B | -0.13973 |
| 51B -> 66B | 0.11153 |
| 54B -> 66B | 0.16481 |
| 55B -> 66B | 0.55417 |
| 56B -> 66B | 0.61455 |
| 57B -> 66B | -0.13966 |
| 61B -> 66B | -0.18492 |
| 64B -> 66B | -0.12045 |

Excited State 18: 2.106-A  5.4678 eV  226.75 nm  f=0.0024  <S**2>=0.859

| Transition | Value |
|------------|-------|
| 66A -> 67A | 0.13507 |
| 43B -> 66B | 0.26294 |
| 42B -> 66B | 0.24036 |
| 45B -> 66B | 0.33961 |
| 46B -> 66B | -0.28339 |
| 50B -> 66B | 0.27153 |
| 51B -> 66B | -0.10625 |
| 52B -> 66B | 0.30699 |
| 53B -> 66B | 0.43632 |
| 54B -> 66B | -0.36982 |
| 59B -> 66B | 0.14373 |
| 62B -> 67B | 0.14822 |
| 65B -> 67B | -0.11373 |

Excited State 19: 2.151-A  5.9710 eV  207.64 nm  f=0.0018  <S**2>=0.906

| Transition | Value |
|------------|-------|
| 41B -> 66B | 0.26294 |
| 42B -> 66B | 0.24036 |
| 45B -> 66B | 0.33961 |
| 46B -> 66B | -0.28339 |
| 50B -> 66B | 0.27153 |
| 51B -> 66B | -0.10625 |
| 52B -> 66B | 0.30699 |
| 53B -> 66B | 0.43632 |
| 54B -> 66B | -0.36982 |
| 59B -> 66B | 0.14373 |
| 62B -> 67B | 0.14822 |
| 65B -> 67B | -0.11373 |

Excited State 20: 2.207-A  6.1384 eV  201.98 nm  f=0.0023  <S**2>=0.967

| Transition | Value |
|------------|-------|
| 61A -> 67A | 0.10155 |
| 40B -> 66B | -0.29064 |
| 43B -> 66B | 0.47438 |
| 44B -> 66B | -0.34797 |
| 45B -> 66B | 0.21840 |
| 46B -> 66B | -0.20010 |
| 50B -> 66B | -0.30662 |
| 51B -> 66B | 0.12750 |
| 52B -> 66B | -0.40828 |
| 53B -> 66B | 0.24077 |
| Transition | E (eV)  | λ (nm)  | f | S^2 |
|------------|---------|--------|----|-----|
| 62B -> 67B | -0.11735 |        |    |     |

**3'SC(S1)**

| Excited State | E (eV)  | λ (nm)  | f | S^2 |
|---------------|---------|--------|----|-----|
| 1: 2.037 Å    | 1.2612  | 983.04 | 0.0048 | 0.788 |
| 61B -> 66B    | -0.37552 |        |    |     |
| 62B -> 66B    | -0.59218 |        |    |     |
| 63B -> 66B    | -0.27225 |        |    |     |
| 65B -> 66B    | 0.62854  |        |    |     |
| 2: 2.053 Å    | 2.5370  | 488.70 | 0.0033 | 0.804 |
| 53B -> 66B    | -0.10949 |        |    |     |
| 56B -> 66B    | 0.14036  |        |    |     |
| 60B -> 66B    | 0.17586  |        |    |     |
| 61B -> 66B    | 0.69199  |        |    |     |
| 64B -> 66B    | 0.12450  |        |    |     |
| 65B -> 66B    | 0.51300  |        |    |     |
| 3: 2.045 Å    | 2.6908  | 460.78 | 0.0034 | 0.795 |
| 53B -> 66B    | -0.16022 |        |    |     |
| 54B -> 66B    | 0.13841  |        |    |     |
| 60B -> 66B    | 0.28493  |        |    |     |
| 61B -> 66B    | -0.20303 |        |    |     |
| 62B -> 66B    | -0.28924 |        |    |     |
| 63B -> 66B    | 0.17091  |        |    |     |
| 64B -> 66B    | 0.78941  |        |    |     |
| 65B -> 66B    | -0.23405 |        |    |     |
| 4: 2.061 Å    | 3.1589  | 392.50 | 0.0139 | 0.812 |
| 54B -> 66B    | 0.11661  |        |    |     |
| 55B -> 66B    | 0.12316  |        |    |     |
| 56B -> 66B    | -0.34145 |        |    |     |
| 61B -> 66B    | -0.27441 |        |    |     |
| 62B -> 66B    | -0.11823 |        |    |     |
| 63B -> 66B    | 0.79912  |        |    |     |
| 64B -> 66B    | -0.27371 |        |    |     |
| 5: 2.042 Å    | 3.2857  | 377.35 | 0.0014 | 0.793 |
| 51B -> 66B    | -0.10045 |        |    |     |
| 57B -> 66B    | -0.10179 |        |    |     |
| 60B -> 66B    | -0.11972 |        |    |     |
| 61B -> 66B    | -0.33874 |        |    |     |
| 62B -> 66B    | 0.67159  |        |    |     |
| 64B -> 66B    | 0.35438  |        |    |     |
| 65B -> 66B    | 0.49016  |        |    |     |
| 6: 2.185 Å    | 3.4940  | 354.85 | 0.0426 | 0.943 |
| 61A -> 68A    | 0.14687  |        |    |     |
| 62A -> 68A    | 0.18217  |        |    |     |
| 63A -> 67A    | -0.17879 |        |    |     |
| Transition  | Energy  |
|-------------|---------|
| 66A -> 67A  | -0.13059 |
| 66A -> 68A  | -0.11756 |
| 49B -> 66B  | 0.11168  |
| 54B -> 66B  | -0.40072 |
| 55B -> 66B  | -0.44605 |
| 56B -> 66B  | 0.47550  |
| 57B -> 66B  | 0.21343  |
| 61B -> 67B  | -0.25605 |
| 61B -> 67B  | 0.10751  |
| 63B -> 66B  | 0.31725  |

Excited State 7: 2.046 Å 3.8489 eV 322.12 nm f=0.0001 <$S^2> = 0.797$

| Transition  | Energy  |
|-------------|---------|
| 49B -> 66B  | -0.13763 |
| 50B -> 66B  | 0.20956  |
| 51B -> 66B  | 0.23093  |
| 53B -> 66B  | -0.34263 |
| 54B -> 66B  | 0.27182  |
| 55B -> 66B  | -0.18459 |
| 57B -> 66B  | -0.23932 |
| 58B -> 66B  | 0.13503  |
| 59B -> 66B  | -0.14284 |
| 60B -> 66B  | 0.57512  |
| 61B -> 66B  | -0.16551 |
| 62B -> 66B  | 0.23817  |
| 64B -> 66B  | -0.33481 |

Excited State 8: 2.051 Å 4.1493 eV 298.81 nm f=0.0003 <$S^2> = 0.802$

| Transition  | Energy  |
|-------------|---------|
| 49B -> 66B  | 0.10160  |
| 50B -> 66B  | -0.20862 |
| 51B -> 66B  | -0.22644 |
| 53B -> 66B  | 0.57192  |
| 54B -> 66B  | -0.12918 |
| 56B -> 66B  | -0.12663 |
| 57B -> 66B  | 0.15116  |
| 58B -> 66B  | 0.23685  |
| 59B -> 66B  | 0.12809  |
| 60B -> 66B  | 0.62274  |

Excited State 9: 2.068 Å 4.2589 eV 291.12 nm f=0.0004 <$S^2> = 0.819$

| Transition  | Energy  |
|-------------|---------|
| 48B -> 66B  | -0.14441 |
| 49B -> 66B  | 0.11507  |
| 51B -> 66B  | 0.20374  |
| 53B -> 66B  | -0.12608 |
| 55B -> 66B  | 0.16445  |
| 57B -> 66B  | 0.22916  |
| 58B -> 66B  | 0.85351  |
| 60B -> 66B  | -0.20701 |
| Excited State | 10: 2.048 Å | 4.4003 eV | 281.76 nm | f=0.0007 | <S**2>=0.799 |
|---------------|-------------|----------|-----------|----------|--------------|
| 47B -> 66B    | 0.14612     |
| 48B -> 66B    | -0.33461    |
| 49B -> 66B    | 0.36365     |
| 51B -> 66B    | 0.30559     |
| 54B -> 66B    | 0.10859     |
| 55B -> 66B    | 0.15705     |
| 57B -> 66B    | 0.51448     |
| 58B -> 66B    | -0.32004    |
| 59B -> 66B    | -0.40031    |
| 60B -> 66B    | 0.15133     |
| 65B -> 66B    | 0.10725     |

| Excited State | 11: 2.990 Å | 4.4385 eV | 279.34 nm | f=0.0081 | <S**2>=1.985 |
|---------------|-------------|----------|-----------|----------|--------------|
| 61A -> 68A    | 0.28855     |
| 62A -> 68A    | 0.43726     |
| 63A -> 67A    | 0.33434     |
| 63A -> 68A    | 0.20722     |
| 64A -> 67A    | -0.19752    |
| 66A -> 67A    | 0.36980     |
| 66A -> 68A    | -0.20514    |
| 58B -> 66B    | 0.12781     |
| 59B -> 66B    | -0.18199    |
| 61B -> 67B    | 0.20988     |
| 62B -> 67B    | 0.27637     |
| 63B -> 67B    | 0.12681     |
| 65B -> 67B    | -0.26481    |

| Excited State | 12: 2.088 Å | 4.4654 eV | 277.65 nm | f=0.0005 | <S**2>=0.840 |
|---------------|-------------|----------|-----------|----------|--------------|
| 47B -> 66B    | 0.12215     |
| 48B -> 66B    | -0.18226    |
| 50B -> 66B    | 0.15428     |
| 51B -> 66B    | 0.17031     |
| 57B -> 66B    | 0.17200     |
| 58B -> 66B    | -0.19185    |
| 59B -> 66B    | 0.85732     |

| Excited State | 13: 2.068 Å | 5.0359 eV | 246.20 nm | f=0.0014 | <S**2>=0.820 |
|---------------|-------------|----------|-----------|----------|--------------|
| 42B -> 66B    | -0.15138    |
| 47B -> 66B    | -0.33117    |
| 48B -> 66B    | 0.27144     |
| 49B -> 66B    | -0.37077    |
| 51B -> 66B    | -0.22820    |
| 53B -> 66B    | -0.26749    |
| 54B -> 66B    | 0.17086     |
| 57B -> 66B    | 0.65111     |

| Excited State | 14: 2.873 Å | 5.1203 eV | 242.14 nm | f=0.0042 | <S**2>=1.814 |
|---------------|-------------|----------|-----------|----------|--------------|
| Transition  | Value     |
|------------|-----------|
| 61A -> 67A | 0.33881   |
| 62A -> 67A | 0.58344   |
| 63A -> 67A | 0.25217   |
| 63A -> 68A | -0.31264  |
| 64A -> 68A | 0.19241   |
| 66A -> 67A | -0.33498  |
| 66A -> 68A | -0.38109  |
| 62B -> 68B | -0.12323  |
| 65B -> 68B | 0.11993   |

**Excited State 15:** 2.083 A 5.1302 eV 241.67 nm f=0.0011 <S**2>=0.835

| Transition  | Value     |
|------------|-----------|
| 41B -> 66B | 0.10736   |
| 42B -> 66B | -0.10400  |
| 43B -> 66B | 0.22578   |
| 45B -> 66B | 0.37641   |
| 46B -> 66B | 0.50323   |
| 47B -> 66B | 0.43739   |
| 50B -> 66B | 0.22278   |
| 51B -> 66B | -0.27983  |
| 52B -> 66B | -0.20159  |
| 54B -> 66B | 0.28220   |
| 55B -> 66B | -0.11613  |

**Excited State 16:** 2.331 A 5.2868 eV 234.52 nm f=0.0623 <S**2>=1.108

| Transition  | Value     |
|------------|-----------|
| 61A -> 67A | 0.10377   |
| 62A -> 67A | 0.17429   |
| 63A -> 68A | 0.35061   |
| 64A -> 68A | -0.19009  |
| 66A -> 67A | -0.16018  |
| 66A -> 68A | 0.34215   |
| 42B -> 66B | -0.10244  |
| 45B -> 66B | -0.12381  |
| 53B -> 66B | 0.25275   |
| 54B -> 66B | 0.37815   |
| 55B -> 66B | 0.15153   |
| 56B -> 66B | 0.45129   |
| 61B -> 66B | -0.11162  |
| 61B -> 68B | -0.14105  |
| 62B -> 68B | -0.18825  |
| 65B -> 68B | 0.17834   |

**Excited State 17:** 2.385 A 5.3379 eV 232.27 nm f=0.0240 <S**2>=1.172

| Transition  | Value     |
|------------|-----------|
| 62A -> 67A | -0.13218  |
| 62A -> 68A | -0.14702  |
| 63A -> 67A | 0.11709   |
| 63A -> 68A | -0.36842  |
| 64A -> 67A | -0.10574  |
| Transition   | Energy   |
|--------------|----------|
| 64A -> 68A   | 0.18340  |
| 66A -> 67A   | 0.31320  |
| 66A -> 68A   | -0.28368 |
| 53B -> 66B   | 0.18014  |
| 54B -> 66B   | 0.28481  |
| 55B -> 66B   | 0.12030  |
| 56B -> 66B   | 0.50002  |
| 61B -> 68B   | 0.13707  |
| 62B -> 68B   | 0.19720  |
| 65B -> 68B   | -0.19895 |

Excited State 18: 2.409-A
5.4462 eV 227.65 nm f=0.1498 <S**2>=1.201

| Transition   | Energy   |
|--------------|----------|
| 62A -> 67A   | 0.18839  |
| 63A -> 67A   | 0.47459  |
| 63A -> 68A   | 0.10622  |
| 64A -> 67A   | -0.23160 |
| 66A -> 67A   | 0.38035  |
| 66A -> 68A   | 0.22436  |
| 42B -> 66B   | 0.14048  |
| 45B -> 66B   | 0.15333  |
| 54B -> 66B   | -0.32742 |
| 55B -> 66B   | -0.14789 |
| 56B -> 66B   | 0.18286  |
| 61B -> 67B   | -0.16202 |
| 62B -> 67B   | -0.23994 |
| 63B -> 67B   | -0.12210 |
| 65B -> 67B   | 0.25340  |

Excited State 19: 2.069-A
5.6420 eV 219.75 nm f=0.0043 <S**2>=0.820

| Transition   | Energy   |
|--------------|----------|
| 45B -> 66B   | 0.25819  |
| 49B -> 66B   | -0.12940 |
| 51B -> 66B   | -0.12361 |
| 53B -> 66B   | -0.25253 |
| 54B -> 66B   | -0.34425 |
| 55B -> 66B   | 0.72058  |
| 56B -> 66B   | 0.26557  |
| 60B -> 66B   | 0.17286  |

Excited State 20: 2.126-A
5.9459 eV 208.52 nm f=0.0003 <S**2>=0.880

| Transition   | Energy   |
|--------------|----------|
| 40B -> 66B   | 0.19836  |
| 41B -> 66B   | -0.30164 |
| 42B -> 66B   | 0.19691  |
| 43B -> 66B   | 0.48693  |
| 44B -> 66B   | 0.19552  |
| 49B -> 66B   | -0.42957 |
| 50B -> 66B   | 0.23779  |
| 51B -> 66B   | 0.31633  |
Table S4. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of $3$, $3'$, $\text{TS}$, and $4$ in hartree computed at the PCM(water)/(TD-)$\omega$B97XD/6-311++G(d,p) level of theory.

| compound   | $E$     | ZPVE   | $H$     | $G$     |
|------------|---------|--------|---------|---------|
| $3(S_0)$   | $-772.200043$ | 0.336145 | $-771.849724$ | $-771.902342$ |
| $3(S_1)$   | $-772.024240$ | 0.330859 | $-771.678357$ | $-771.732814$ |
| $3'(S_0)$  | $-772.188675$ | 0.335160 | $-771.838757$ | $-771.892762$ |
| $3'(S_1)$  | $-772.013289$ | 0.329769 | $-771.668068$ | $-771.723800$ |
| $\text{TS}(S_0)$ | $-772.151188$ | 0.332666 | $-771.804330$ | $-771.857011$ |
| $\text{TS}(S_1)$ s.p. | $-772.034317$ | n.a.   | n.a.   | n.a.   |
| $4(S_0)$   | $-695.722207$ | 0.306650 | $-695.402073$ | $-695.454941$ |
| $4(S_1)$   | $-695.620555$ | 0.303339 | $-695.303578$ | $-695.356520$ |

Table S5. Conical intersection optimization scan for $4(S_0)$ formation in hartree computed at the (TD-)$\omega$B97X/6-311++G(d,p) level of theory using ORCA 4.2.0.

| Item            | Geometry convergence | Tolerance | Converged |
|-----------------|----------------------|-----------|-----------|
| Energy change   | 0.0125993207         | 0.0000050000 | NO        |
| E diff. (CI)    | 0.0053210067         | 0.0001000000 | NO 3.3 kcal mol$^{-1}$ |
| RMS gradient    | 0.0069959798         | 0.0001000000 | NO        |
| MAX gradient    | 0.0535645244         | 0.0003000000 | NO        |
| RMS step        | 0.0188608384         | 0.0020000000 | NO        |
| MAX step        | 0.2071330471         | 0.0040000000 | NO        |
| Max(Bonds)      | 0.0478               | Max(Angles) | 3.30      |
| Max(Dihed)      | 11.87                | Max(Improp) | 0.00      |
### Table S6. Geometries of 3, 3', TS, and 4 in Cartesian coordinates in Å computed at the PCM(water)/(TD-B)87XD/6-311++G(d,p) level of theory.

|   | 3(S0) | 3(S0) | 3(S0) | 3(S0) |
|---|------|------|------|------|
| 6 | -2.619962000 | 0.936194000 | -1.541115000 |
| 6 | -3.353689000 | 0.334400000 | -0.337393000 |
| 6 | -2.334823000 | -0.236073000 | 0.655523000 |
| 6 | -1.516082000 | -1.334427000 | -0.035649000 |
| 6 | -0.751072000 | -0.720567000 | -1.229701000 |
| 6 | -1.773569000 | -0.143109000 | -2.223765000 |
| 6 | -1.693317000 | 2.055895000 | -1.060384000 |
| 6 | -1.397629000 | 0.885734000 | 1.125734000 |
| 6 | 0.163352000 | 0.373857000 | -0.713762000 |
| 6 | -0.642371000 | 1.494680000 | -0.082754000 |
| 6 | 1.912303000 | 3.418723000 | -3.133119000 |
| 6 | 1.536491000 | 0.057559000 | -0.380632000 |
| 6 | 1.913592000 | -1.306688000 | -0.226545000 |
| 6 | 3.115048000 | -1.698651000 | 0.338602000 |
| 6 | 4.036883000 | -0.742457000 | 0.761624000 |
| 6 | 3.756777000 | 0.599562000 | 0.535724000 |
| 6 | 2.578311000 | 0.996823000 | -0.076826000 |
| 8 | 2.483042000 | 2.346581000 | -0.349619000 |
| 6 | -3.350930000 | 1.336829000 | -2.255212000 |
| 1 | -3.965027000 | 1.102304000 | 0.153733000 |
| 1 | -4.037066000 | -0.455346000 | -0.672651000 |
| 1 | -2.860140000 | -0.659268000 | 1.519704000 |
| 1 | -2.176972000 | 2.137610000 | -0.390416000 |
| 1 | -0.808706000 | -1.780962000 | 0.673152000 |
| 1 | -1.784730000 | -1.497579000 | -1.741647000 |
| 1 | -1.252007000 | 0.273367000 | -3.092330000 |
| 1 | -2.418925000 | -0.951197000 | -2.591704000 |
| 1 | -1.208020000 | 2.517524000 | -1.913648000 |
| 1 | -2.278430000 | 2.835661000 | -0.553734000 |
| 1 | -1.975161000 | 1.674408000 | 1.629974000 |
| 1 | -0.673805000 | 0.500594000 | 1.852362000 |
| 1 | -0.002241000 | 2.286133000 | 0.287064000 |
| 1 | 1.993128000 | 4.223809000 | -3.631316000 |
| 1 | 1.194741000 | -2.075513000 | -0.488370000 |
| 1 | 3.324261000 | -2.756808000 | 0.471251000 |
| 1 | 4.971934000 | -1.035870000 | 1.225745000 |
| 1 | 4.477713000 | 1.370579000 | 0.786131000 |
| 1 | 2.311124000 | 2.516069000 | -1.254736000 |

**Table S6.** Geometries of 3, 3', TS, and 4 in Cartesian coordinates in Å computed at the PCM(water)/(TD-B)87XD/6-311++G(d,p) level of theory.
|   | 2.088489000 | 1.522285000 | -0.522893000 |
|---|-------------|-------------|--------------|
| 6 | 1.028666000 | -0.405984000 | -1.727214000 |
| 6 | 0.069685000 | 0.387018000 | 0.480485000 |
| 6 | 0.757903000 | 0.820101000 | -0.842180000 |
| 6 | -0.016505000 | 1.592541000 | 1.283490000 |
| 6 | -1.374823000 | -0.075507000 | 0.258922000 |
| 6 | -1.838865000 | -1.358724000 | 0.549549000 |
| 6 | -3.147810000 | -1.750260000 | 0.289752000 |
| 6 | -4.038234000 | -0.840218000 | -0.265522000 |
| 6 | -3.628625000 | 0.463683000 | -0.503528000 |
| 6 | -2.323232000 | 0.853939000 | -0.217648000 |
| 6 | -2.022904000 | 2.168633000 | -0.401904000 |
| 1 | 3.957199000 | 1.064875000 | 0.466001000 |
| 1 | 3.797850000 | -0.305363000 | -1.618444000 |
| 1 | 4.002266000 | -1.339285000 | -0.201507000 |
| 1 | 2.194939000 | -2.225945000 | -1.666078000 |
| 1 | 2.022506000 | -2.498181000 | 0.827124000 |
| 1 | 0.459251000 | -2.431816000 | 0.033633000 |
| 1 | 0.538474000 | -0.971804000 | 2.104950000 |
| 1 | 2.175821000 | 0.916763000 | 2.181477000 |
| 1 | 2.992784000 | -0.637491000 | 2.029832000 |
| 1 | 1.910463000 | 2.416208000 | 0.077956000 |
| 1 | 2.551410000 | 1.844142000 | -1.462453000 |
| 1 | 1.453802000 | -0.066140000 | -2.677415000 |
| 1 | 0.091591000 | -0.923438000 | -1.959861000 |
| 1 | 0.104372000 | 1.509327000 | -1.380653000 |
| 1 | -0.400140000 | 1.359358000 | 2.134106000 |
| 1 | -1.171496000 | -2.081135000 | 0.997505000 |
| 1 | -3.464233000 | -2.760375000 | 0.521781000 |
| 1 | -5.058469000 | -1.133029000 | -0.487063000 |
| 1 | -4.317989000 | 1.207592000 | -0.886624000 |
| 1 | -1.249373000 | 2.366306000 | 0.152326000 |

| 3(S2) |
|-------|
| 6     |
| 0.3031351000 | 0.505052000 | -0.012337000 |
| 6     |
| 3.197768000 | -0.827434000 | -0.756111000 |
| 6     |
| 1.832315000 | -1.518081000 | -0.874611000 |
| 6     |
| 1.266796000 | -1.772357000 | 0.526982000 |
| 6     |
| 1.072070000 | -0.433212000 | 1.267161000 |
| 6     |
| 2.446659000 | 0.250272000 | 1.386145000 |
| 6     |
| 2.075554000 | 1.404034000 | -0.807195000 |
| 6     |
| 0.853040000 | -0.619974000 | -1.643853000 |
| 6     |
| 0.101144000 | 0.488666000 | 0.496716000 |
| 6     |
| 0.700093000 | 0.725832000 | -0.919726000 |
| 8     |
| 0.089431000 | 1.832896000 | 1.109599000 |
| 6     |
| -1.328180000 | 0.020469000 | 0.463808000 |
| 6     |
| -1.856390000 | -1.197863000 | 0.957699000 |
| 6     |
| -3.053520000 | -1.712780000 | 0.428225000 |
| 6     |
| -3.839939000 | -1.004314000 | -0.520120000 |
| 6     |
| -3.532314000 | 0.358757000 | -0.717400000 |
| 6     |
| -2.314264000 | 0.857398000 | -0.212717000 |
|   |       |       |       |       |
|---|-------|-------|-------|-------|
| 8 | -2.11122 | 2.16470 | 0.289804 |
| 1 | 4.003595 | 0.998073 | 0.085047 |
| 1 | 3.619319 | -0.649576 | -1.752174 |
| 1 | 3.896991 | -1.476894 | -0.217180 |
| 1 | 1.943247 | -2.471730 | -1.399830 |
| 1 | 1.959819 | -2.391584 | 1.107088 |
| 1 | 0.330190 | -2.326401 | 0.447690 |
| 1 | 0.666631 | -0.617425 | 2.268763 |
| 1 | 2.361901 | 1.191029 | 1.935196 |
| 1 | 3.114845 | -0.402760 | 1.958029 |
| 1 | 1.979161 | 2.379720 | -0.327133 |
| 1 | 2.471354 | 1.570516 | -1.815801 |
| 1 | 1.222501 | -0.438040 | -2.658604 |
| 1 | -0.120046 | -1.114800 | -1.734375 |
| 1 | 0.023886 | 1.369344 | -1.490123 |
| 1 | -0.215525 | 1.727676 | 2.017498 |
| 1 | -1.321097 | -1.783216 | 1.694825 |
| 1 | -3.391897 | -2.687680 | 0.768261 |
| 1 | -4.754205 | -1.433890 | -0.906232 |
| 1 | -4.250921 | 1.064620 | -1.120281 |
| 1 | -1.278530 | 2.365422 | 0.204937 |

$3'(S_0)$

|   |       |       |       |       |
|---|-------|-------|-------|-------|
| 6 | -3.09559 | 0.271846 | -0.373440 |
| 6 | -3.217436 | 0.321386 | -1.036577 |
| 6 | -1.81576 | 0.597791 | -1.597765 |
| 6 | -1.076848 | 1.587822 | -0.688163 |
| 6 | -0.936867 | 0.980263 | 0.722257 |
| 6 | -2.346478 | 0.708043 | 1.280278 |
| 6 | -2.295917 | -1.576253 | 0.314937 |
| 6 | -1.012342 | -0.707969 | -1.654335 |
| 6 | -0.104697 | 0.333936 | 0.679499 |
| 6 | -0.890362 | -1.305473 | -0.244378 |
| 8 | -0.094450 | -0.942274 | 1.979397 |
| 6 | 1.374977 | -0.209047 | 0.230977 |
| 6 | 2.041567 | -1.417171 | -0.038649 |
| 6 | 3.369047 | -1.490398 | -0.418378 |
| 6 | 4.108627 | -0.319567 | -0.537332 |
| 6 | 3.505626 | 0.885984 | -0.243281 |
| 6 | 2.165380 | 0.952374 | 0.157600 |
| 8 | 1.761965 | 2.220268 | 0.455157 |
| 1 | -4.091838 | -0.463424 | 0.783601 |
| 1 | -3.752141 | -0.375180 | -1.692238 |
| 1 | -3.797430 | 1.250795 | -1.005510 |
| 1 | -1.896110 | 1.024093 | 2.602074 |
| 1 | -1.631687 | 2.529172 | -0.617893 |
| 1 | -0.104054 | 1.821738 | -1.128869 |
| 1 | -0.485650 | 1.685930 | 1.432745 |
| 1 | -2.275378 | 0.308261 | 2.294084 |
| 1 | -2.883377 | 1.660972 | 1.338364 |
| 1 | -2.226189 | 2.024500 | 1.308665 |
|   |      |      |      |
|---|------|------|------|
|   | -2.796900000 | -2.299726000 | -0.337902000 |
|   | -1.513622000 | -1.431607000 | -2.305627000 |
|   | -0.020308000 | -0.523063000 | -2.079236000 |
|   | -0.361740000 | -2.257220000 | -0.296960000 |
|   | 0.479483000  | 0.423272000  | 2.547857000  |
|   | 1.493653000  | -2.344170000 | 0.066612000  |
|   | 3.821616000  | -2.457451000 | 0.616806000  |
|   | 5.148687000  | -0.345629000 | -0.842103000 |
|   | 4.058246000  | 1.816861000  | -0.300506000 |
|   | 0.859421000  | 2.227630000  | 0.776595000  |
|   | -3.039237000 | -0.139118000 | 0.074436000  |
|   | -2.882258000 | 0.158536000  | -1.423278000 |
|   | -1.391258000 | 0.291498000  | 1.764789000  |
|   | -0.777232000 | 1.432622000  | -0.945380000 |
|   | -0.918984000 | 1.132095000  | 0.556707000  |
|   | -2.413916000 | 0.997700000  | 0.893941000  |
|   | -2.316224000 | -1.449936000 | 0.411494000  |
|   | -0.661195000 | -1.013601000 | -1.418194000 |
|   | -0.177975000 | -0.181253000 | 0.921335000  |
|   | -0.822592000 | -1.317999000 | 0.078121000  |
|   | -0.430266000 | -0.538070000 | 2.298084000  |
|   | 1.332950000  | -0.137672000 | 0.738170000  |
|   | 2.075892000  | -1.360340000 | 0.750827000  |
|   | 3.009723000  | -1.585276000 | -0.256645000 |
|   | 3.443834000  | -0.548750000 | -1.132933000 |
|   | 3.074007000  | 0.762866000  | -0.830050000 |
|   | 2.102090000  | 0.967467000  | 0.158031000  |
|   | 2.034873000  | 2.198260000  | 0.679542000  |
|   | -4.101083000 | -0.228327000 | 0.324589000  |
|   | -3.332106000 | -0.647071000 | -2.015047000 |
|   | -3.408379000 | 1.085069000  | -1.680643000 |
|   | -1.273018000 | 0.506628000  | -2.831303000 |
|   | -1.283402000 | 2.378315000  | -1.168079000 |
|   | 0.270939000  | 1.565300000  | -1.234236000 |
|   | -0.519132000 | 1.964278000  | 1.146970000  |
|   | -2.540352000 | 0.807080000  | 1.962292000  |
|   | -2.912962000 | 1.946015000  | 0.665689000  |
|   | -2.448713000 | -1.696562000 | 1.467300000  |
|   | -2.739293000 | -2.273591000 | -0.175004000 |
|   | -1.076876000 | -1.843587000 | -1.999820000 |
|   | 0.399656000  | -0.933427000 | -1.679124000 |
|   | -0.306951000 | -2.249683000 | 0.324268000  |
|   | 0.157289000  | 0.000753000  | 2.836621000  |
|   | 1.774575000  | -2.178109000 | 1.395931000  |
|   | 3.409000000  | -2.587098000 | -0.390086000 |
|   | 4.185589000  | -0.754991000 | -1.893773000 |
|   | 3.645391000  | 1.613705000  | -1.188053000 |
|   | 1.437221000  | 2.187292000  | 1.439752000  |
|   |   |   |   |   |
|---|---|---|---|---|
| 6 | -2.967272000 | 0.602205000 | -0.258292000 |   |
| 6 | -3.360304000 | -0.626338000 | 0.573406000 |   |
| 6 | -2.096892000 | -1.415280000 | 0.942843000 |   |
| 6 | -1.387047000 | -1.873018000 | -0.334266000 |   |
| 6 | -0.959896000 | -0.628733000 | -1.167231000 |   |
| 6 | -2.235042000 | 0.156288000 | -1.530734000 |   |
| 6 | -2.038921000 | 1.496688000 | 0.570132000 |   |
| 6 | -1.137767000 | -0.530206000 | 1.746991000 |   |
| 6 | -0.038992000 | 0.187396000 | -0.295698000 |   |
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| 8 | 0.121074000 | 1.939582000 | -1.297437000 |   |
| 6 | 1.373459000 | -0.118308000 | 0.497865000 |   |
| 6 | 1.888673000 | -1.354742000 | 0.249331000 |   |
| 6 | 3.196322000 | -1.715217000 | 0.621677000 |   |
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| 6 | 3.605452000 | 0.433940000 | 1.746991000 |   |
| 6 | 2.747697000 | 0.863430000 | 0.922377000 |   |
| 8 | 1.914793000 | 2.085659000 | 0.497865000 |   |
| 1 | -3.863923000 | 1.163319000 | -0.536604000 |   |
| 1 | -3.885788000 | -0.311355000 | 1.481405000 |   |
| 1 | -4.043060000 | -1.265873000 | 1.538310000 |   |
| 1 | -2.366449000 | -2.922460000 | 1.538310000 |   |
| 1 | -2.054734000 | -2.473950000 | 0.956576000 |   |
| 1 | -0.526036000 | -2.494435000 | -0.807860000 |   |
| 1 | -0.441935000 | -0.947039000 | -2.073658000 |   |
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| 1 | -2.877311000 | -0.499388000 | -2.127175000 |   |
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| 6 | 0.765211000 | 1.131425000 | 0.278660000 |   |
| 6 | 2.581119000 | -0.313743000 | 1.278099000 |   |
| 6 | 3.494395000 | 0.019868000 | 0.088506000 |   |
| 6 | 2.643828000 | 0.286424000 | -1.163014000 |   |
| 6 | 1.803307000 | -0.951270000 | 1.485415000 |   |
| 6 | 0.881141000 | -1.293869000 | -0.289651000 |   |
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| 6 | 1.623294000 | 0.851554000 | 1.533545000 |   |
| 6 | 1.698357000 | 1.464797000 | -0.506546000 |   |
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| 6       | -1.396181000  | -0.169954000  | -0.133585000  |
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| 1       | 2.179399000   | 1.763551000   | 1.775123000   |
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1  0.975241000  -2.339898000  0.948637000
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1  1.236273000  2.261212000  -1.055839000
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