Supplementary material

Protection against chemical submission: Naked-eye detection of γ-hydroxybutyric acid (GHB) in soft drinks and alcoholic beverages

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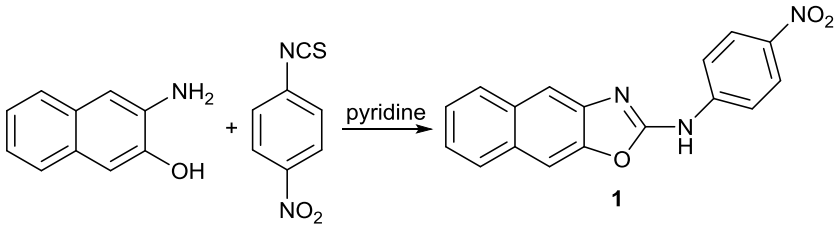
Material and methods

The reagents employed in the synthesis were acquired in Sigma Aldrich and used without further purification. ^{1}H NMR, ^{13}C NMR and 19F NMR spectra were registered with Bruker Avance 300 MHz, 400 MHz or 500 MHz spectrophotometers, all of them referenced to solvent peak, DMSO(d_6) o THF(d_8). UV-Vis spectra were registered with a Shimadzu UV-2600 spectrophotometer, using a cuvette with 1 cm of path length. Fluorescent measures were carried out with a FluoroMax-4 Spectrofluorometer, employing a cuvette with 1 cm of path length. Mass spectrometry spectra were carried out with a TripleTOFTM 5600 LC/MS/MS System, with 2 gas sources (both to 35 psi), 450 °C and ion gas voltage of 5500 V. Origin 2020 was the program to plot tritations.

Synthesis of compounds

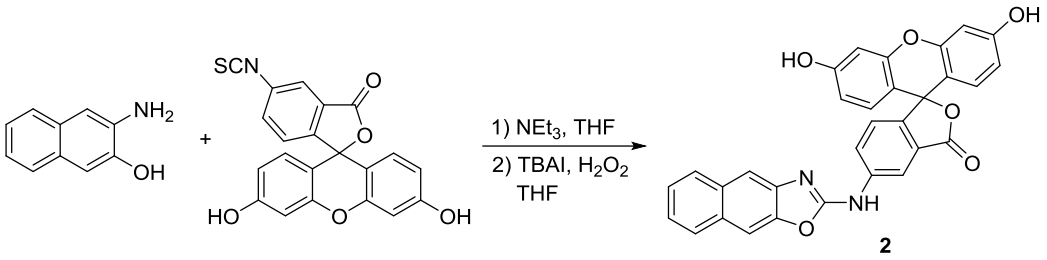
Synthesis compound **1**



Scheme S1. Synthesis pathway to prepare compound **1**

In 13 mL of pyridine, 202 mg (1.256 mmol) of 3-amino-2-naphtol were mixed with 191 mg (1.047 mmol) of 4-nitrophenyl isothiocyanate under argon atmosphere for 8 h at room temperature. Then, the solvent was removed to vacuum and the solid was solved in 35 mL of ethyl acetate. The organic phased was washed with 20 mL of an acidic aqueous solution (pH 5), 20 mL of $NaHCO_3$ (sat) and 20 mL of NaCl (sat), dried over anhydrous $MgSO_4$ and filtered. The solvent was removed and the crude was purified by chromatography column using a 6:4 Hexane:AcOEt mixture as eluent and silica gel as solid support. A yellow lightly orange was obtained in a 35 % of yield. ^{1}H NMR (300 MHz, DMSO) δ 11.64 (s, 1H), 8.34 (d, *J* = 9.4 Hz, 2H), 8.13 – 7.94 (m, 6H), 7.62 – 7.27 (m, 2H). ^{13}C NMR (75 MHz, DMSO) δ 158.36, 146.77, 144.62, 142.03, 141.66, 131.28, 129.96, 127.75, 127.68, 125.39, 124.64, 124.50, 117.67, 113.39, 105.06. HRMS: m/z calculated for $C_{17}H_{12}N_3O_3$ (M + H): 306.0879; found: 306.0877 $[M + H]^+$.

Synthesis compound **2**



Scheme S2. Synthesis pathway to prepare compound **2**

45 mg (0.283 mmol) of 3-amino-2-naphtol were mixed with 98 mg (0.283 mmol) of fluorescein-5-isothiocyanate in 3 mL of THF. Next, 50 µL (0.359 mmol) of NEt_3 were added and the stirring was kept for 16 h to room temperature. Then, 34 µL (0.565 mmol) of H_2O_2 30 % and 1 mg (0.003 mmol) of tetrabutylammonium iodide were added and the mixture was sitirred for 24 h. Finally, the solvent was remove and the product was isolated as an orange powder without further purification in a 79 % of yield. ^{1}H NMR (500 MHz, DMSO) δ 8.56 (d, *J* = 2.1 Hz, 1H), 8.08 – 7.93 (m, 6H), 7.60 – 7.39 (m, 2H), 7.30 (d, *J* = 8.4 Hz, 1H), 6.87 (s, 1H), 6.76 – 6.59 (m, 5H), 6.55 (dd, *J* = 8.7, 2.4 Hz, 3H). ^{13}C NMR (126 MHz, DMSO) δ 151.47, 146.96, 139.19, 131.32, 129.74, 129.26, 128.03, 127.70, 127.54, 124.91, 124.52, 124.22, 112.74, 109.99, 104.71, 102.26. HRMS: m/z calculated for $C_{31}H_{19}N_2O_6$ (M + H): 515.1243; found: 515.1239 $[M + H]^+$.

NMR Spectra

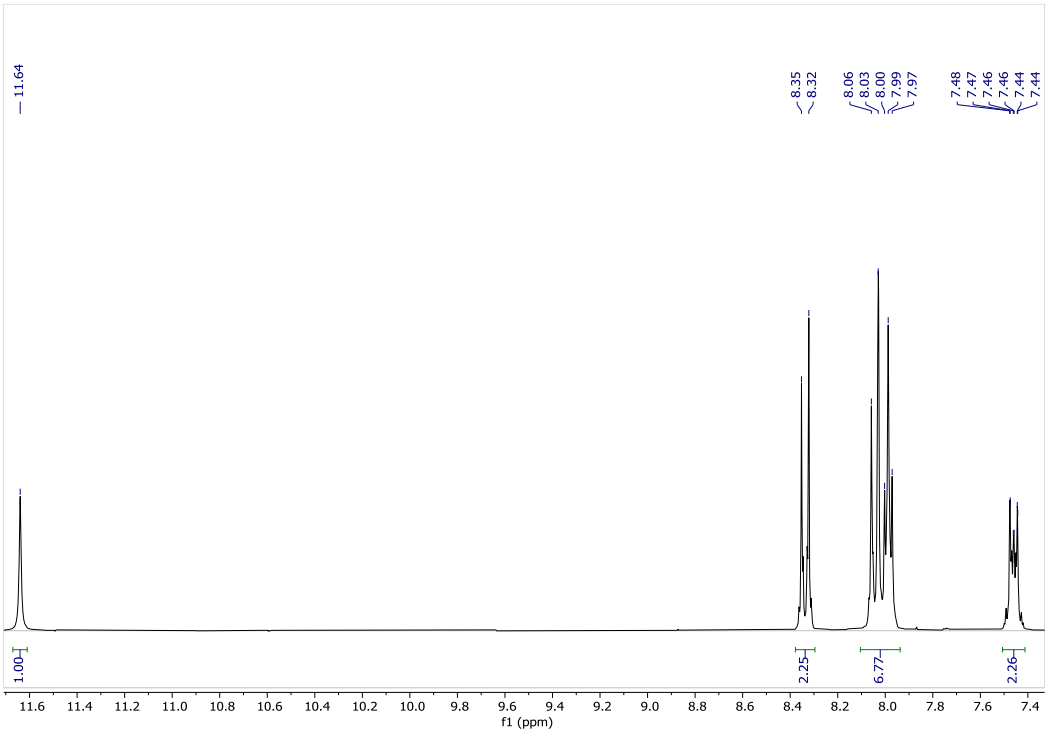


Figure S1. ^{1}H NMR of compound **1**

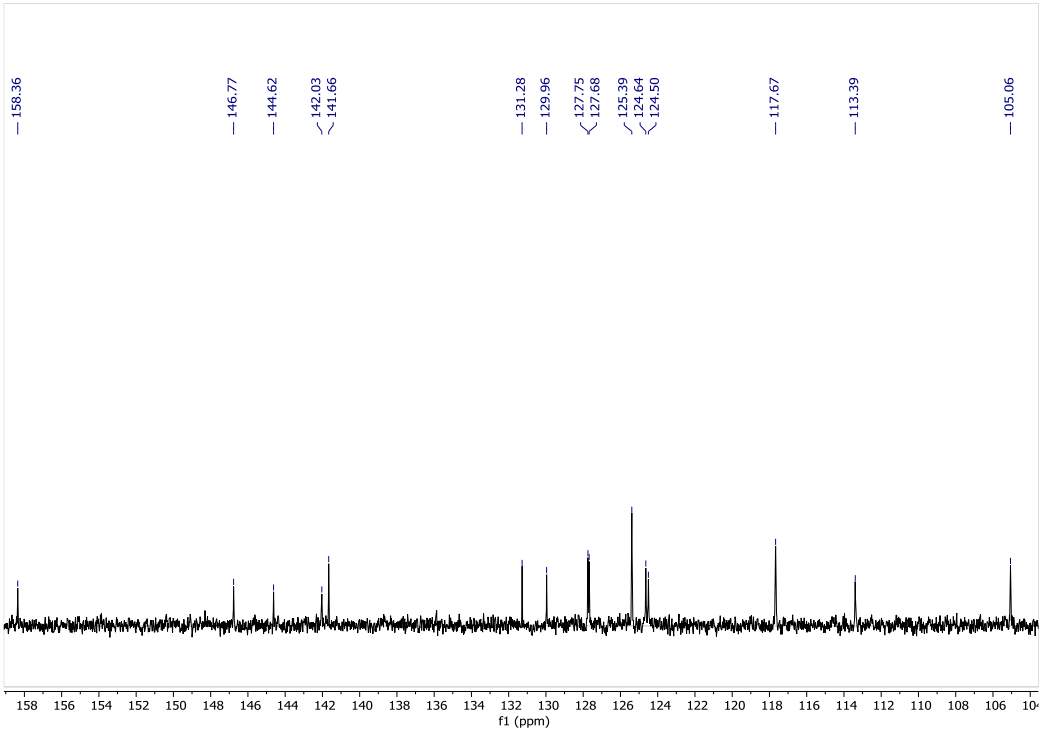


Figure S2. ^{13}C NMR of compound **1**

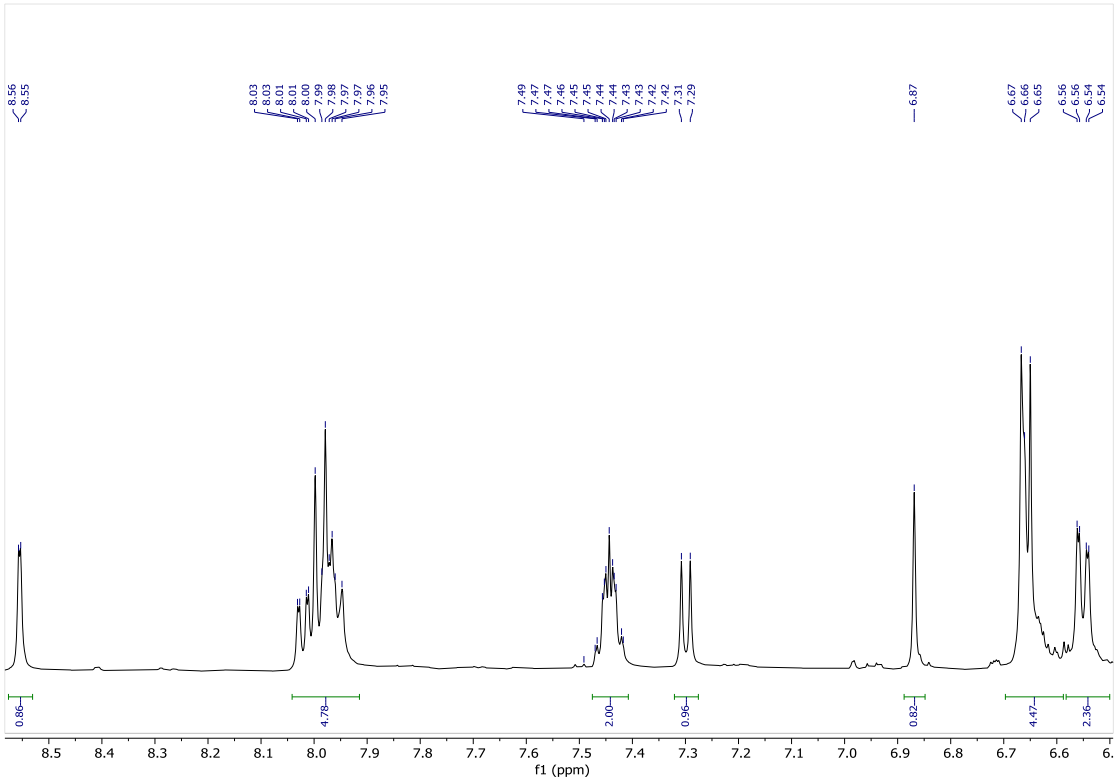


Figure S3. ^{1}H NMR of compound **2**

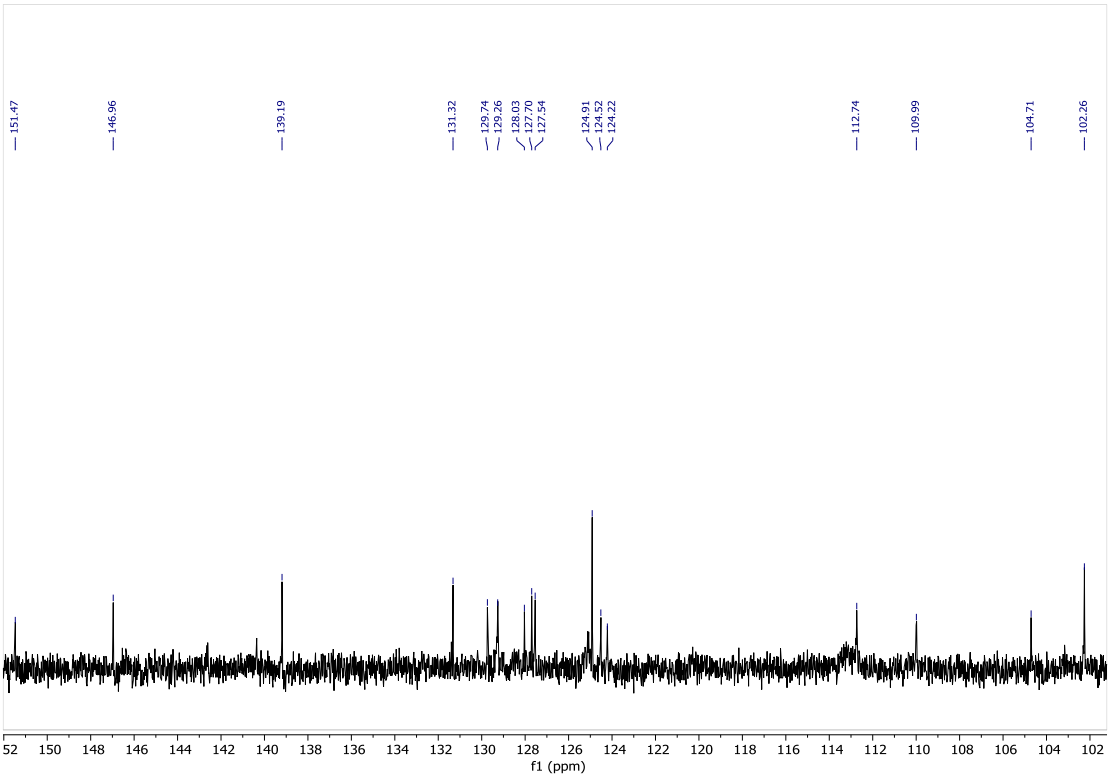


Figure S4. ^{13}C NMR of compound **2**

Mass Spectroscopy Spectra

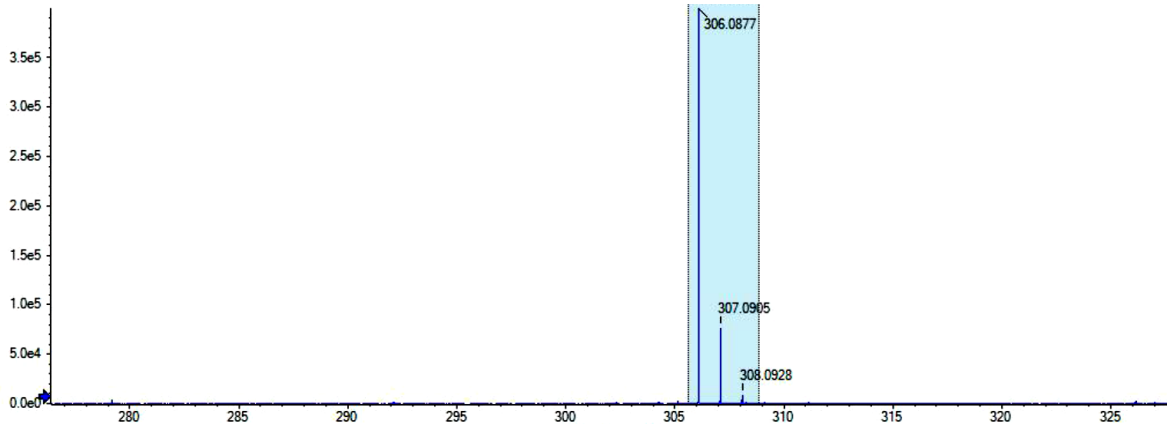


Figure S5. Mass Spectrum compound **1**

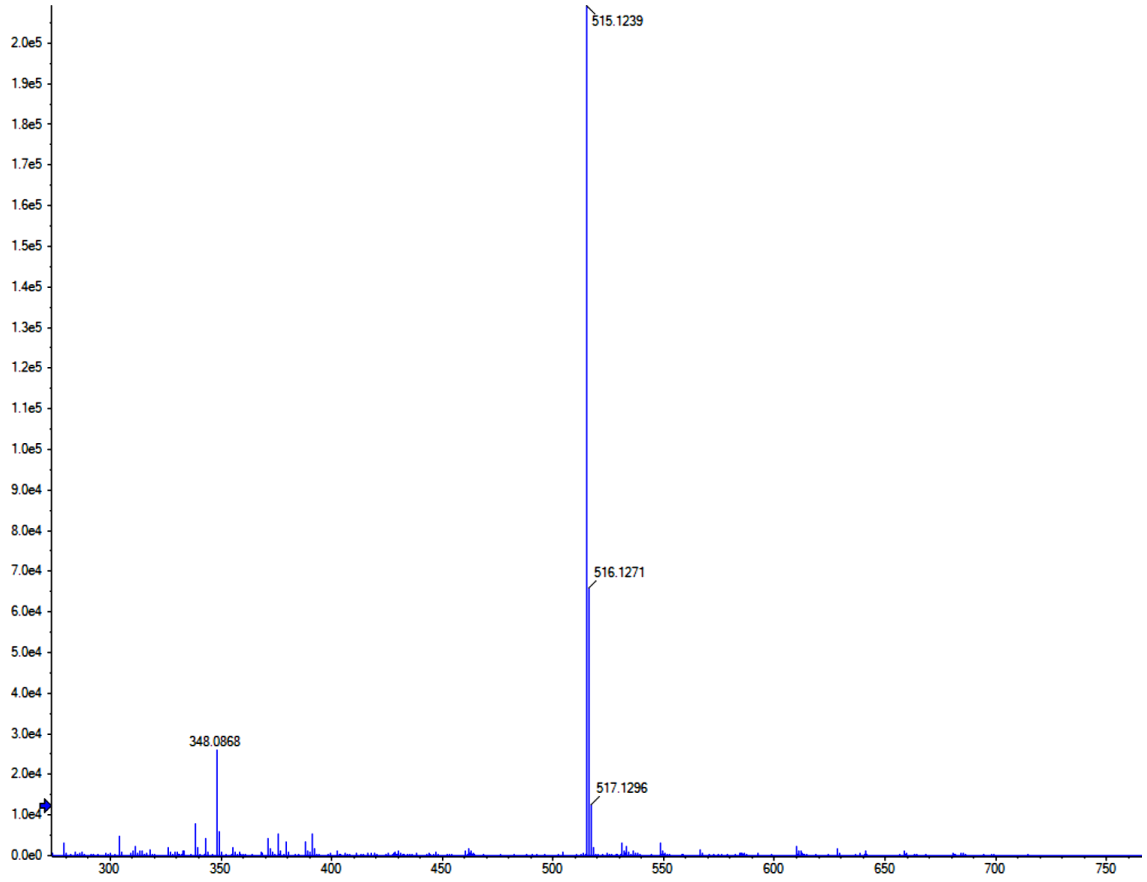


Figure S6. Mass Spectrum of compound **2**

Comparision methods

Table S1. Comparison of methods reported in literature

Derivative	**BODIPY [1]**	**BODIPY [2]**	**Ir Complex [3]**	**Oxazole**
Interaction	Hydrogen bonds	Hydrogen bonds	Not specified	Deprotonation
Signal change	Turn-off fluorescence	Turn-on fluorescence	Turn-off fluorescence	Chromogenic (**1**) or enhancement fluorescence (**2**)
Determination	Mixture 1:1 sample with sensor solution	Extraction with DCM and addition of water	Samples and sensor solved in water	Previous pretreatment with base
C_F sensor (μM)	50	10	2.5	50
C_F GHB (mg/mL)	5	10	0.15	0.045

References

[1] D. Zhai, Y. Qiao, E. Tan, W. Xu and Y-T. Chang, Chem Commun., 2014, 50, 2904-2906.

[2] D. Zhai, B. K. Agrawalla, P. S. F. Eng, S-C. Lee, W. Xua and Y-T. Chang, Chem Commun., 2013, 49, 6170-6172.

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Tritations

NMR titration

A solution 10 mM of **1** and 200 mM of NaGHB were prepared in DMSO-*d6*. 400 µL were taken from the solution of **1** and increasing amounts of NaGHB were added, until a total volume of 500 µL.

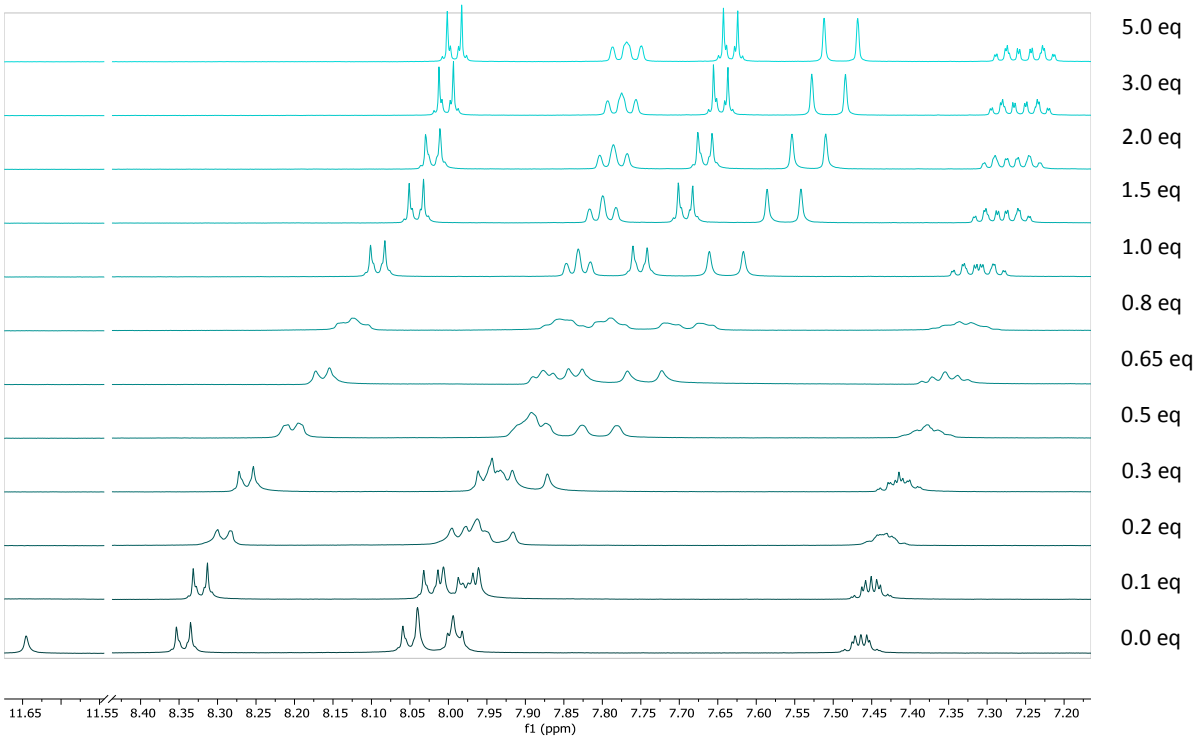


Figure S7. ^{1}H NMR studies of compound **1** in DMSO-*d6* with increasing amounts of GHB

UV titration

In a 3 mL cuvette (1 cm of path of length), 2475 µL of DMSO were mixed with 25 µL of sensor from a 1 mM solution in DMSO. After that, increasing quantities of NaGHB were added from a 2,5 mM solution of NaGHB in DMSO until arriving to saturation point.

Fluorescence titration

In a 3 mL cuvette (1 cm of path of length), 2475 µL of DMSO were mixed with 25 µL of sensor from a 1 mM solution in DMSO. Then, increasing quantities of NaGHB were added from a 2,5 mM solution of GHB in DMSO until arriving to saturation point. The samples were irradiated with a wavelength of 490 nm.

Aqueous media titration

In a 3 mL cuvette (1 cm of path of length), 2350 µL of DMSO were mixed with 125 µL of deionized water and 25 µL of sensor from a 1 mM solution in DMSO. After that, increasing quantities of NaGHB were added from a 2,5 mM solution of NaGHB in DMSO until arriving to saturation point.

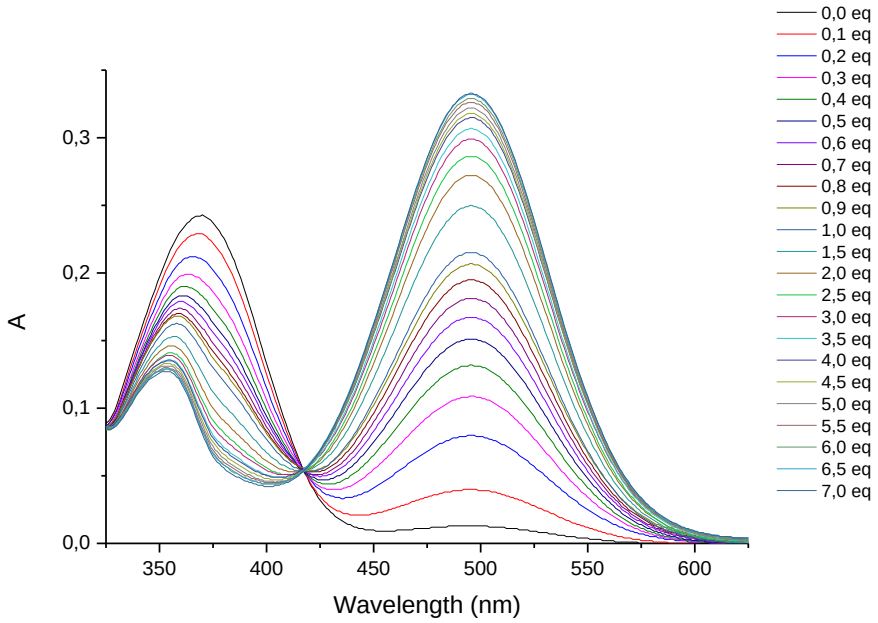


Figure S8. Titration of GHB with compound **1** in DMSO:H_2O 95:5 media (10 µM of **1**)

Comparision with other bases

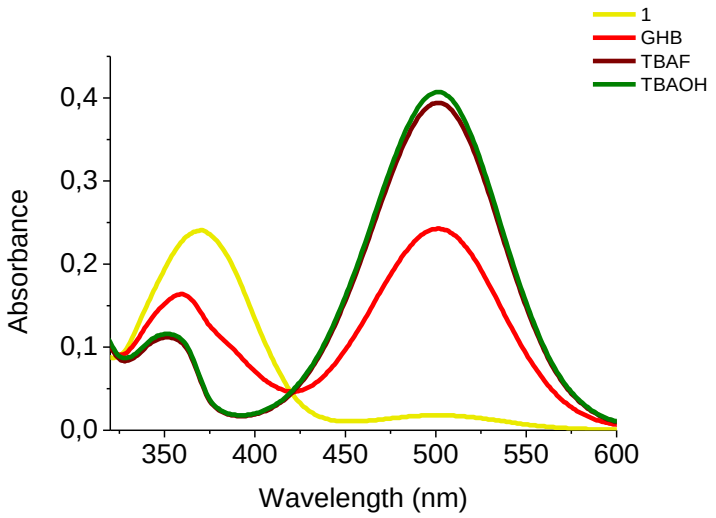


Figure S9. UV-Vis spectra variation of **1** (yellow) in DMSO with 0.5 eq of: GHB (red), TBAF (garnet) and TBAOH (green)

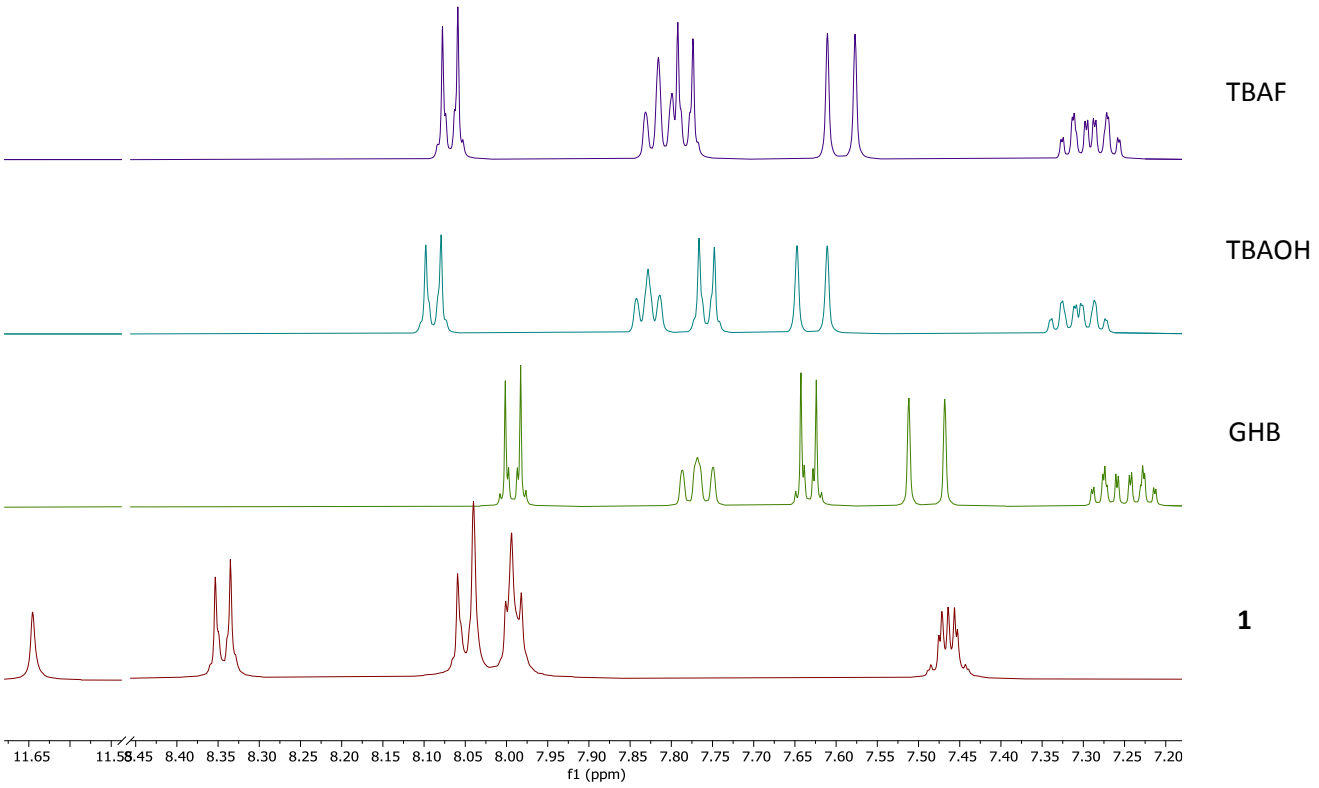
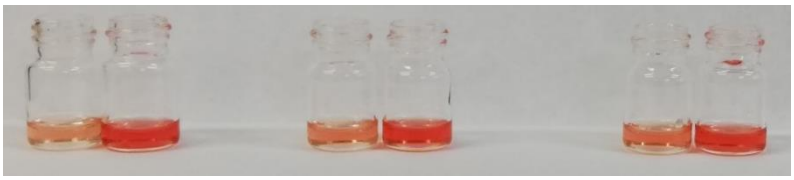


Figure S10. ^{1}H NMR spectra variation of **1** (red) in DMSO-*d6* with 0.5 eq of: GHB (green), TBAF (blue) and TBAOH (purple)

Real Samples Analysis

In first place, the drinks were contaminated with NaGHB in a 12 mM concentration (except Gin tonic whose concentration was 20 mM). After that, an aliquot of 100 µL was taken and mixed with 100 µL of $NaHCO_3$ 0.4 mM, at room temperature. Then, 30 µL of this solution was taken and mixed with 50 µL of sensor (1 mM in DMSO) and 920 µL of DMSO. Colour or fluorescence changes were observed immediately. The same process was followed for the samples without GHB.



Rum Gin Vodka

Figure S11. Colour change observed with alcoholic drinks using compound 1

Nestea Beer

Figure S12. Colour change observed with soft drinks using compound 1

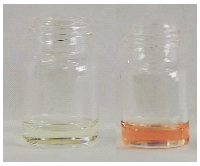


Figure S13. Colour change observed with a beverage (Gin Tonic) using compound 1

Rum Gin Vodka

Figure S14. Fluorescent changes observed in compound **2** with real samples (alcoholic drinks)

Nestea Beer

Figure S15. Fluorescent changes observed in compound **2** with real samples (soft drinks)

Figure S16. Colour change observed with a beverage (Gin Tonic) using compound **2**

Theoretical calculations

Complete reference for Gaussian

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

The following Supporting Information section, which contains the details of computational calculations performed in this work, has been structured in the following subsections (which, in turn, has its own bibliographic references included at the end):

- Computational methods. In this section, computational details about the geometrical optimizations, the vertical excitation energy analysis and pK_a calculations are given.
- Potential energy surface (PES) full-search. In this section, geometry and relative energies of compounds **1** and **1-** as well as their conformers **1'** and **1'-** and tautomers **1t** and **1t'** together with the the transition states leading to their interconversion will be described.
- Boltzmann distribution of species.
- Complete TD-DFT vertical excitation energies analysis. This will be done over all stationary points described in the previous sections, namely **1**/**1-**, **1'**/**1'**- and **1t**/**1t'**. Different DFT functionals and basis sets will be included used to predict the UV-Vis spectra starting from B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometries.
- pK_a calculations of the acid-base conjugate pairs **1**/**1-**, **1'**/**1'**- and **1t**/**1t'** through a thermodynamic cycle.
- Annex I: XYZ cartesian coordinates of the minima and TS geometries found along the PES.
- Annex II: Excitation energies, oscillator strengths, spin and spatial symmetry, the S^2 and the largest coefficients in the CI expansion for all TD-DFT vertical excitation energies computed.

Computational Methods

In order to gain insight in the behavior of **1** in presence of GHB, DFT calculations have been carried out using Gaussian09 rev. D01 program package [4] and GaussView 5 [5] was employed to visualize the results. In this sense, structures of **1** and **1-** were modeled. The geometrical optimization was performed using Becke3-Lee-Yang-Parr hybrid functional (B3LYP) [6] with the split-valence triple-ζ 6-311++G(2df,2p) basis set [7]. To take into account the effect of the solvent, DMSO, PCM solvation model was used [8]. Frequency calculations were performed over optimized structures to properly characterize minima and transition structures (none and a single imaginary frequency, respectively).

On the other hand, to explore the electronic transitions responsible for the UV-Vis spectra, vertical excitation energies were computed over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometries through single-point TD-DFT [9] calculations (30 states, singlets only) in solution using non-equilibrium formalism at the same theory level. Geometry details as well as a full-search performed over the potential energy surface (PES) can be found in the corresponding section of this Electronic Supplementari Information. Finally, to compute pK_a of the acid-base conjugate pairs **1**/**1-** and **1'**/**1'**, the calculation scheme used by Ho via the thermodynamic cycle (MP2-TC) was reproduced [10]. In this scheme, a previous systematic conformer search was performed in both gas and solution phases to locate the global minimum energy structure of each species at the M06-2X/6-31+G(d) [11] level using an ultrafine grid. Solution phase calculations were carried within the SMD solvation model [12] using the default settings in Gaussian09. The corresponding thermal corrections to the Gibbs free energy were computed using a factor of 0.967 to scale the frequencies [13] and using the ideal gas molecular partition functions in conjunction with the rigid-rotor quasiharmonic oscillator (RR-QHO) approximation. In the QHO [14] approximation, vibrational frequencies that were lower than 100 cm-1 were raised to 100 cm^{-1} due to the breakdown of the harmonic oscillator model for low frequency vibrational modes. This was done with Goodvibes script [15] which, in addition, allowed to apply over the standard state calculations in Gaussian (1 atm and 298.15 K conditions) the appropriate corrections to ensure that all solution phase pK_as are computed at a standard state of 1 mol/L. Single-point calculations at (RO)MP2/GTMP2Large theory level was performed on the M06-2X/6-31G+(d) optimised geometries. To compute the pK_a of each acid-base pair, we have employed the proton free energy $AG^*_s(H^+)$ of -273.3 [16] kcal/mol, that is consistent with the parametrisation of the SMD model.

[4] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[5] GaussView, Version 5, Roy Dennington, Todd Keith, and John Millam, Semichem Inc., Shawnee Mission, KS, 2009.

[6] a) A.D. Becke, J.Chem.Phys. 98 (1993) 5648-5652. b) C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785-789. c) S.H. Vosko, L. Wilk, M. Nusair, Can. J. Phys. 58 (1980) 1200-1211. d) P.J. Stephens, F.J. Devlin, C.F. Chabalowski, M.J. Frisch, J.Phys.Chem. 98 (1994) 11623-11627.

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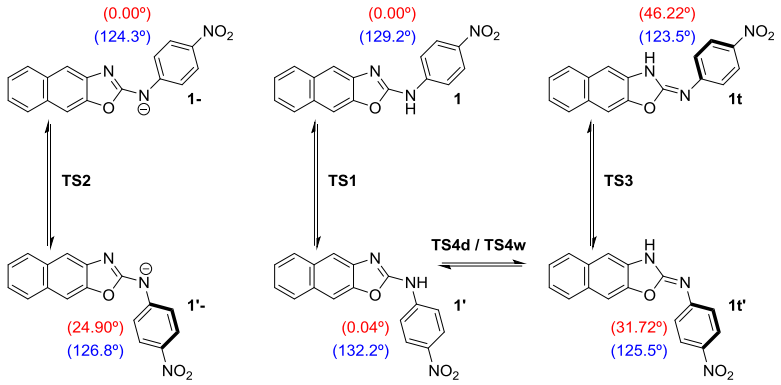
[16] C. P. Kelly, C. J. Cramer, D. G. Truhlar, "Single-ion solvation free energies and the normal hydrogen electrode potential in methanol, acetonitrile, and dimethyl sulfoxide", J Phys Chem B., 111 (2007) 408-422.

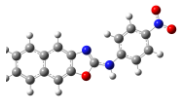
Potential energy surface (PES) full-search

Firstly, an exploration of the PES of the conformational and tautomeric equilibria involving compounds **1** and **1-** was performed at B3LYP/6-311++G(2df,2p)/PCM(DMSO) level. This search included the conformers **1'** and **1'-** obtained from **1** and **1-** through the rotation of the C-N bond between the naphthoxazole ring and *p*-aminonitrobenzene moiety and the tautomeric forms **1t** and **1t'**, with the proton on the naphthoxazole moiety instead of the nitrogen beteen the naphthoxazole moiety and *p*-aminonitrobenzene moiety (see Scheme S3). The transition state (TS) between each conformer/tautomer pair was also located and characterized.

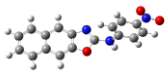


Scheme S3. Scheme of the species located along the PES search of **1** and **1-** conformational and tautomeric equilibria and the TSs connecting them. In TS4, letters d and w indicate direct or water-mediated mechanism, respectively. In red, dihedral angle between naphthoxazole and *p*-aminonitrobenzene rings. In blue, C-N-C angle between two system rings.

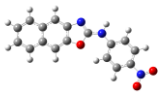
The lowest energy geometries of **1**, **1'** and **1-** turned out to be almost planar (see dihedral angles between naphthoxazole and *p*-aminonitrobenzene rings depicted in red in Scheme S3) while **1'-**, **1t** and **1t'** had 24.9, 46.2 and 31.7 degrees between its two ring systems. The C-N-C angle between two system rings in the stationary points found, depicted in blue in Scheme S3 gives us an idea of the partial C-N double bond character between the naphthoxazole ring and the nitrogen. In this sense, at **1-**, **1'-**, **1t** and **1t'** optimized geometries this angle takes the values 124.3, 126.8, 123.5 and 125.5º, respectively, while at **1** and **1'**, this angle is 129.2 and 132.2 º, respectively. The dihedral angle formed between the N-$C_{p\text{-aminonitrobenzene}}$ bond and the naphthoxazol moiety plane at the corresponding TSs of the conformational equilibria between **1/1'**, **1-/1'-** and **1t/1t'** geometries, namely **TS1**, **TS2** and **TS3**, takes the values 87.2, 93.1 and 95.0º, respectively. Regarding the TS connecting **1'** and **1t'** through a tautomerization process (that has been studied both from the theoretical and experimental point of view on 2-aminobenzothiazole derivatives, see refs. [17] and [18]), one has to take into account that there is no equivalent TS between geometries **1** and **1t** since in these compounds hydrogen atom carried by the nitrogen atom between the two ring systems is not in a *syn*-coplanar rearrangement with the oxazol nitrogen atom (antarafacial shift). From that point, the location of the only transition state between **1'** and **1t'** can be made through a direct 1,3-hydride shift process through **TS4d** and through a process catalyzed by two water molecules (see reference [17] for the different catalysis with 1 to 3 water molecules) through **TS4w**. In the case of the latter, to evaluate the enegy barrier of the water-catalized process, two molecular complexes had to be optimized, both formed by **1'** and **1t'** with two water molecules, namely **MC1' and MC1t'**. In the case of **TS4d**, the $N_{naphthoxazol}\cdots H\cdots N_{exocyclic}$ bond distances were 1.331 and 1.418 angstroms, respectively, while the $N_{naphthoxazol}\cdots H$ forming-bond and $H\cdots N_{exocyclic}$ breaking-bond distances at **TS4w** were 1.126 and 1.121 angstroms, respectively. Geometries for all above discussed stationary points are depicted in Figure S17, although further details can be obtained at Annex I, were XYZ atomic coordinates are collected.



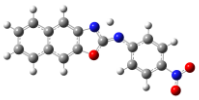
1



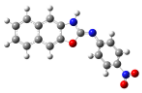
TS1



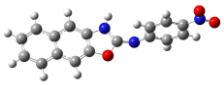
1'



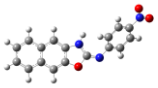
TS4d



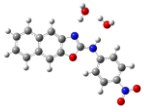
1t'



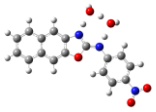
TS3



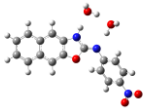
1t



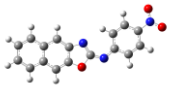
MC1'



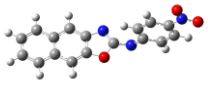
TS4w



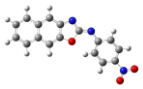
MC1t'



1-



TS2



1'-

Figure S17. Geometries of the stationary points and the TSs found along the PES. For further details about these geometries (distances, angles, …) please see Annex I, where XYZ atomic coordinates are depicted.

Once some remarkable geometrical details of the stationary points found along the PES had been shown, it is time to discuss the energy aspects of the PES. Among the six computed geometries, the most stable conformers are **1**, **1-** and **1t'** (1.5, 1.8 and 1.0 kcal/mol more stable respectively than their corresponding conformers **1'** and **1'-** and **1t**). In addition, the interconversion between conformers **1** and **1'**, **1-** and **1'-** and **1t** and **1t'** takes place through the corresponding TSs, namely **TS1**, **TS2** and **TS3**, that are located 8.2, 5.9 and 9.7 kcal/mol above the most stable structure of each pair. Regarding the tautomeric equilibria between **1'**and **1t'** that connects **1**/**1'** and **1t**/**1t'** rotamer pairs, direct and water-catalyzed processes were studied. In the direct process without catalysis, the energy barrier is 52.7 kcal/mol from the the most stable conformer **1t'**. The water-catalyzed process, taking as the energy reference the molecular complexes **MC1'** and **MC1t'**, the energy barrier is 17.4 kcal/mol. Therefore, the catalysis of two water molecules lowers the barrier of the process by 35.3 kcal/mol. Taking into account the thermal corrections to enthalpies and entropies (computed at 25 ^{o}C and 1 atm and scaling the frequencies by a factor of 0.96 [10]) to yield the Gibbs free energy of each stationary point, do not modify the conclusions discussed above. In fact, the exothermic or endothermic character of each conformational or tautomeric process is kept over the Gibbs PES and the value of the free energy barriers of the different processes through **TS1**, **TS2**, **TS3** is lower than 1.1 kcal/mol. The major variation comes with **TS4d** and **TS4w** were the free barriers are lowered to 50.35 kcal/mol and 14.33 kcal/mol but, as can be seen, conclusions are the same as previously stated. The absolute electronic and free Gibbs energies, together with the relative energies of every process are collected in Table S2 and the free energy profile is depicted in Figure S18.

Table S2. Absolute electronic and free Gibbs energies (computed at 298.15 K and 1 atm and scaling frequencies by 0.96) of the stationary points found along the PES full-search. Please, note that compound **1** has been used as reference in the relative electronic and free Gibbs energies. *In the case of water-catalyzed process through **TS4w**, the most stable molecular complex, **MC1'**, has been used as reference to compute the barrier of the tautomerization process. Boltzmann distribution according to the Eq. 1 has been included.

Structure	**E** (hartree)	**ΔE** (kcal/mol)	**G** (hartree)	**ΔG** (kcal/mol)	**Boltzmann distribution** (%)
1	-1044,6466	0,00	-1044,4518	0,00	89.92
TS1	-1044,6335	8,23	-1044,4386	8,27	
1'	-1044,6442	1,53	-1044,4495	1,43	8.03
TS4d	-1044,5602	54,20	-1044,3715	50,35	
1t'	-1044,6417	3,07	-1044,4481	2,33	1.76
TS3	-1044,6262	12,79	-1044,4316	12,67	
1t	-1044,6401	4,08	-1044,4463	3,41	0.28
MC1'	-1197,6037	0,00*	-1197,3695	0,00*	
TS4w	-1197,5760	17,36	-1197,3467	14,33	
MC1t'	-1197,6007	1,88	-1197,3674	1,31	
1-	-1044,1788	0,00	-1043,9979	0,00	96.91
TS2	-1044,1694	5,90	-1043,9866	7,07	
1'-	-1044,1760	1,80	-1043,9946	2,04	3.09

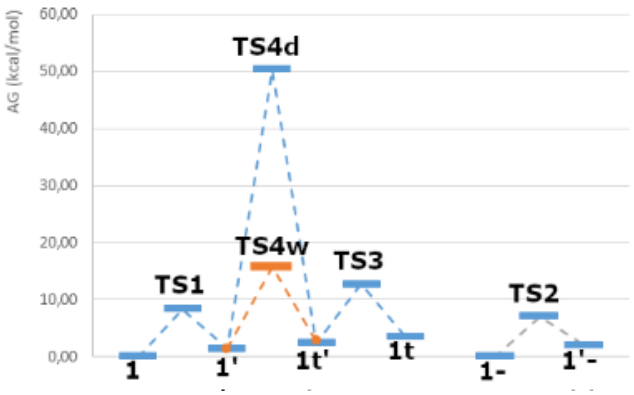


Figure S18. Free energy profile of the different conformational/tautomerization processes found along the PES. Please, note that **MC1'** has moved over compound **1'** (and **MC1t'** over **1t'**) to show the difference in the free energy profile between the direct non-catalyzed process through **TS4d** and the water-catalyzed process through **TS4w**.

[17] D. H. Reid, Organic Compounds of Sulphur, Selenium, and Tellurium, Volume 2, Chemical Society, 1973. ISBN 0851862691.

[18] Wazzan, N., Safi, Z., Al-Barakati, R. et al. DFT investigation on the intramolecular and intermolecular proton transfer processes in 2-aminobenzothiazole (ABT) in the gas phase and in different solvents. Struct Chem 31, 243–252 (2020).

Boltzmann distribution of species

Considering that the temperature of an alcoholic beverage may be between 5 and 25 °C and that the acid-base reaction is considerably faster than the conformational changes and tautomerization reactions, we analyze the relative abundance using the Boltzmann distribution equation 1 on the relative free energies at 298.15 K (see below) of the protonated compounds **1** and **1'** and its corresponding tautomers, **1t** and **1t'**, respectively. In the same way, considering that in presence of GHB, the deprotonation of **1** occurs, the free energy of conformers **1-** and **1'-** was taken and equation 1 was also applied to them at the same temperature. The results, collected in Table S2, showed that the population of **1** and **1-** is around 90 and 97%, respectively**,** of the species present and therefore they can be considered the main responsible for the shape of the UV-Vis spectra in absence and in presence of GHB, respectively. Anyway, the maxima of simulated UV-Vis bands of **1'**, **1t**, **1t'** and **1'-** differ a few nanometers from **1** and **1-** and therefore would only result in a slight broadening of the experimental bands (see later).

Complete TD-DFT vertical excitation energies analysis

Starting from the B3LYP/6-311++(2df,2p)/PCM(DMSO) optimized geometries for all the stationary points found along the PES, namely **1**, **1'**, **1t'**, **1t**, **1-** and **1'-**, single-point TD-DFT calculations at the same theory level were performed in DMSO solution using non-equilibrium formalism which are the ones presented in the main communication. Further single-point TD-DFT calculations in DMSO

solution using B3LYP/6-311++(2df,2p)/PCM(DMSO) optimized geometries were also made using different hybrid DFT functionals (X3LYP [19], PBE0 [20] and CAM-B3LYP [21]) as well as B3LYP functional combined with different triple-ζ quality basis sets as Ahlrichs and coworkers Def2TZVPD [22-23] and Truhlar and Papajak "calendar" basis set jul-cc-pV(T+d)Z [24] that were downloaded from www.basissetexchange.org [25] for the H, C, N and O elements for comparative purposes. In all calculations submitted, the state of interest was the first one and only the first 30 singlet excited states were considered using keywords root=1, nstates=30, singlets. Excitation energies, oscillator strengths, spin and spatial symmetry, the $<S^2>$ and the largest coefficients in the CI expansion for all TD-DFT calculations classified by DFT functional and basis set used have been collected in Annex II.

From all the TD-DFT calculations computed by Gaussian09, GaussView can generate UV-Vis plots using the excitation energies and the oscillator strength for each excited state. Collection of the TD-DFT UV-Vis plots for absorbance values ranging from 250 to 650 nm for compounds **1**, **1'**, **1t'**, **1t**, **1-** and **1'-** together with that obtained experimentally for compound **1** and compound **1** in presence of GHB (scaling the simulated spectra absorbance to fit that found experimentally taking the absorbance value of the highest band allows us to compare different DFT functionals (B3LYP, X3LYP, PBE0 and CAM-B3LYP) and several triple-ζ quality basis sets (6-311++(2df,2p), Def2TZVPD and jul-cc-pV(T+d)Z) with the same DFT functional (B3LYP) in Figures S17 to Figures S22. Oscillator strengths for each TD-DFT UV-Vis plots have been ommited for the sake of simplicity and only absorbances (in arbitrary units) have been plotted.

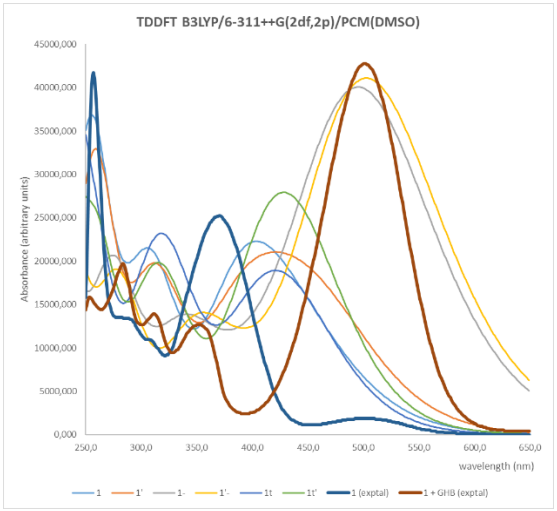


Figure S19. Single-point TDDFT B3LYP/6-311++(2df,2p)/PCM(DMSO) over B3LYP/6-311++(2df,2p)/PCM(DMSO) geometry.

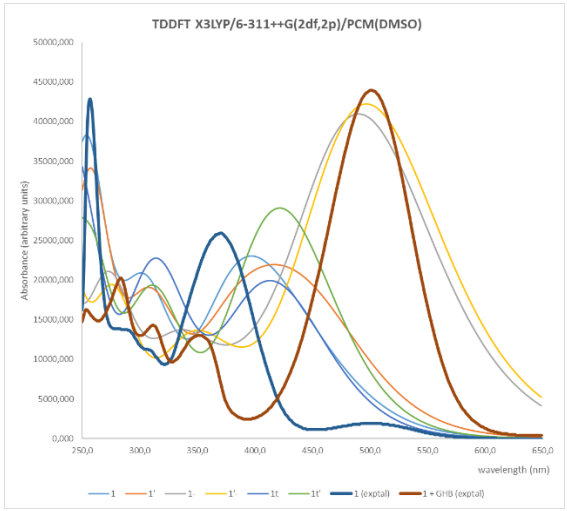


Figure S20. Single-point TDDFT X3LYP/6-311++(2df,2p)/PCM(DMSO) over B3LYP/6-311++(2df,2p)/PCM(DMSO) geometry.

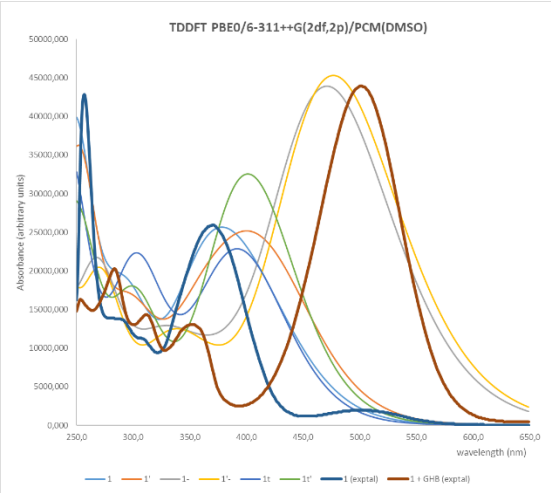


Figure S21. Single-point TDDFT PBE0/6-311++(2df,2p)/PCM(DMSO) over B3LYP/6-311++(2df,2p)/PCM(DMSO) geometry.

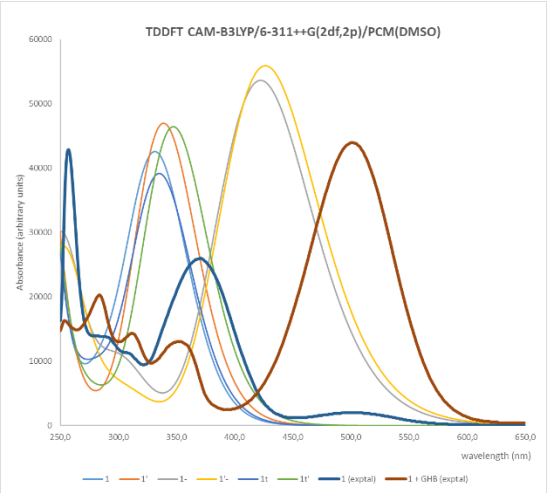


Figure S22. Single-point TDDFT CAM-B3LYP/6-311++(2df,2p)/PCM(DMSO) over B3LYP/6-311++(2df,2p)/PCM(DMSO) geometry.

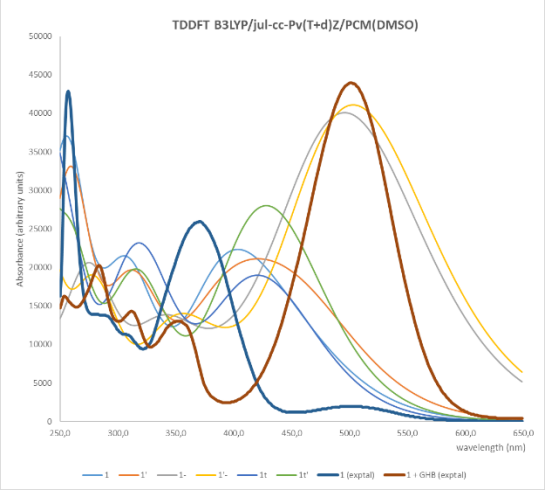


Figure S23. Single-point TDDFT B3LYP/jul-cc-Pv(T+d)Z/PCM(DMSO) over B3LYP/6-311++(2df,2p)/PCM(DMSO) geometry.

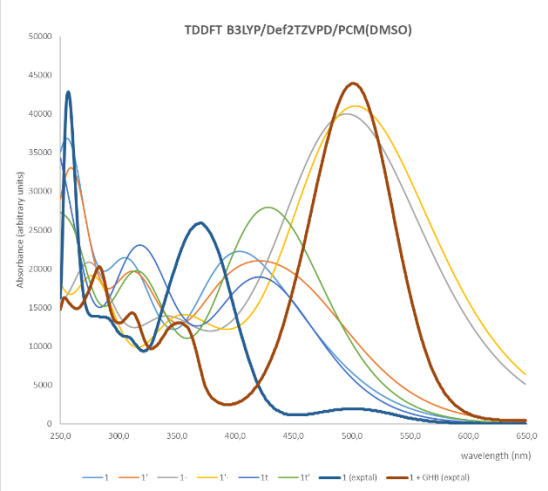


Figure S24. Single-point TDDFT B3LYP/Def2TZVPD/PCM(DMSO) over B3LYP/6-311++(2df,2p)/PCM(DMSO) geometry.

As can be seen, the most accurate overall match between λ_{max} between experimental and simulated UV-Vis plots for all the species depicted are those from TD-DFT B3LYP/6-311++G(2df-2p)/PCM(DMSO) calculations (see Figure S19), although not far away from those reported for X3LYP (second best match, see Figure S20) and PBE0 (see Figure S21) DFT functionals. The functional with the poorest match is CAM-B3LYP (see Figure S22). Also, when comparing the same method (B3LYP) with different basis sets (6-311++G(2df,2p), jul-cc-Pv(T+d)Z and Def2TZVPD, see Figures S19, S23 and S24), almost no difference between the computed UV-Vis plots can be seen.

[19] X. Xu and W. A. Goddard III, “The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties,” Proc. Natl. Acad. Sci. USA, 101 (2004) 2673-77.

[20] C. Adamo and V. Barone, “Toward reliable density functional methods without adjustable parameters: The PBE0 model,” J. Chem. Phys., 110 (1999) 6158-69.

[21] T. Yanai, D. Tew, and N. Handy, “A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP),” Chem. Phys. Lett., 393 (2004) 51-57.

[22] F. Weigend and R. Ahlrichs, “Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy,” Phys. Chem. Chem. Phys., 7 (2005) 3297-305.

[23] F. Weigend, “Accurate Coulomb-fitting basis sets for H to Rn,” Phys. Chem. Chem. Phys., 8 (2006) 1057-65.

[24] E. Papajak, J. Zheng, H. R. Leverentz and D. G. Truhlar, “Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions,” J. Chem. Theory and Comput., 7 (2011) 3027.

[25] A New Basis Set Exchange: An Open, Up-to-date Resource for the Molecular Sciences Community. Benjamin P. Pritchard, Doaa Altarawy, Brett Didier, Tara D. Gibson, Theresa L. Windus. J. Chem. Inf. Model. 2019, 59(11), 4814-4820.

pKa calculations of the acid-base conjugate pairs **1/1-**, **1'/1'-** and **1t/1t'** through a thermodynamic cycle

Finally, in order to find out the interaction between compound **1** and GHB, which is supposed to be an acid-base equilibria to yield compound **1-** as has been pointed out by the experimental data, a thermodynamic cycle was performed to compute the pK_a of both **1/1-** and GHB/GHB^- species in DMSO using the methodology described in the reference [7] of computational methods section in order to evaluate the feasibility of the acid-base process.

To carry on these calculations, first of all, a thorough conformation search over GHB and GHB^- species at M062X/6-31+G(d) level both in gas phase and in solvent (SMD, solvent DMSO) was performed in order to select the most stable conformations. To do so, several starting candidates where the dihedral angles of the C-C and C-O bonds have been rotated were fully optimized until the most stable structure was found (see Figure S25).

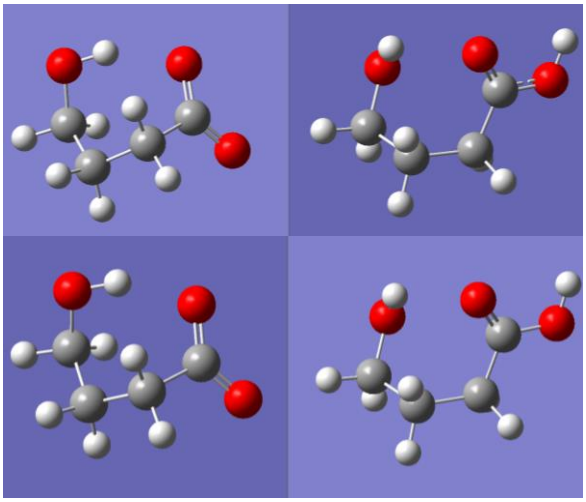


Figure S25. Most stable conformations found for GHB-/GHB pair in DMSO solvent (up) and in gas phase (down).

After this step, an optimization of all stationary points (**1**, **1-**, **1'**, **1'-**, **1t** and **1t'**) was performed at M062X/6-31+G(d) level both in gas phase and in solvent (SMD, solvent DMSO) starting from different geometries to be sure that the lowest energy conformer of the corresponding species had been found. Finally, over the optimized gas phase and solvent geometries of the most stable conformers of the aforementioned species, the corresponding thermal corrections to the Gibbs free energy were computed at 298.15 K and 1 atm using a factor of 0.967 to scale the frequencies using the ideal gas molecular partition functions in conjunction with the rigid-rotor quasiharmonic oscillator (RR-QHO) approximation. This was done with Goodvibes script which, in addition, allowed to apply over the standard state calculations in Gaussian the appropriate corrections to ensure that all solution phase pK_as are computed at a standard state of 1 mol/L.

Finally, over the optimized M062X/6-31+G(d) gas phase geometries, single point calculations at the (RO)MP2/GTMP2Large theory level were performed. Finally, to compute the pK_a of each acid-base pair, we have employed the proton free energy $AG^*_s(H^+)$ of -273.3 kcal/mol.

pK_a was computed through a thermodynamic cycle (TC) using these equations:

$$pK_a = (\Delta G^*_{soln} / RTln(10))$$

Where:

$$\Delta G^*_{soln} = \Delta G^*_{soln}\,(TC) = \Delta E^L_{soln} + \Delta G^{soln,L}_{corr} + G^*_{soln}(H^+) + \Delta E^H_{gas} - \Delta E^L_{gas}$$

Where:

$$\Delta E^X_Y = E^X_Y\,(A^-) - E^X_Y\,(AH)$$

Where X superscript refers to (RO)MP2/GTMP2Large energy when it equals to H (high level calculations) and to M062X/6-31+G(d) energy when it equals to L (low level calculations) and Y subscript refers to gas phase optimized geometry when it equals to "gas" or to solvent phase geometry when it equals to "soln".

And where:

$$\Delta G^{soln,L}_{corr} = \Delta G^{gas}_{corr} - \Delta G^{soln}_{corr}$$

The results of all these calculations are collected in the following Table S3:

Table S3: "Low level" M062X/6-31+G(d) and "high level" M062X/6-31+G(d)/gas phase//(RO)MP2/GTMP2Large calculation results over **1**, **1-**, **1'**, **1'-**, **1t**, **1t'**, GHB and GHB^- minimum-energy geometries.

Species	E^L_{soln} (hartree)	E^H_{gas} (hartree)	E^L_{gas} (hartree)	$G^{soln,L}_{corr}$ (hartree)
1-	-1043,46175841	-1041,7313	-1043,38877017	0,186534
1	-1043,92994532	-1042,2488	-1043,90252410	0,200172
1t	-1043,92255735	-1042,2385	-1043,89252962	0,199082
1'-	-1043,45839550	-1041,7256	-1043,38280982	0,187047
1'	-1043,92680469	-1042,2451	-1043,89906003	0,201494
1t'	-1043,92262142	-1042,2399	-1043,89465108	0,199231
GHB^-	-382,31902611	-381,6959	-382,23164084	0,078718
GHB	-382,78635260	-382,2394	-382,77191902	0,089027

These calculations yield the following pK_as in DMSO for the corresponding acid-base pairs: 10.4 for **1/1-**, 7.4 for **1t/1-**, 10.0 for **1'/1'-**, 8.7 for **1t'/1'-** and 11.3 for GHB/GHB^-. Therefore, taking into account that both the free energy profile and Boltzmann population analysis yields **1** and **1-** as the major products, the difference between the pK_as of **1/1-** and GHB/GHB^- systems (10.4 and 11.3, respectively), which is 0.9 units, accounts for the presence of compound **1-** in equilibrium with **1** in presence of GHB in DMSO solvent and, therefore, for the change in the UV-Vis spectra.

Annex I: XYZ cartesian coordinates of the minima and TS geometries found along the PES

1 – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-6.52154300	1.54768900	0.00000800
C	-6.89086700	0.18433700	0.00000300
C	-5.92785000	-0.79206500	0.00000000
C	-4.54936200	-0.46207600	0.00000100
C	-4.17079800	0.92575400	0.00000600
C	-5.19817000	1.90524000	0.00000900
C	-3.55125900	-1.47452500	-0.00000300
C	-2.26061900	-1.05228600	-0.00000100
C	-1.85957400	0.30283700	0.00000400
C	-2.80210000	1.29772700	0.00000700
C	-0.10041900	-0.88722500	0.00000000
N	-0.46192100	0.35413800	0.00000500
N	1.13605000	-1.44390400	-0.00000100
C	2.37824500	-0.82229200	-0.00000100
C	3.51114400	-1.65366700	0.00000100
C	4.77697200	-1.11122000	0.00000100
C	4.92159400	0.27505000	-0.00000200
C	3.81138500	1.11256600	-0.00000500
C	2.53974100	0.57054700	-0.00000400
N	6.25315400	0.85262200	-0.00000200
O	6.36062400	2.07755900	-0.00002700
O	7.22006700	0.09276400	0.00000800
H	-7.28854100	2.31037600	0.00001000
H	-7.93772700	-0.08759700	0.00000200
H	-6.21035700	-1.83704900	-0.00000400
H	-4.91542700	2.95022300	0.00001200
H	-3.82086600	-2.52103900	-0.00000600
H	-2.52038100	2.34174900	0.00001100
H	1.13655200	-2.45304400	0.00000000
H	3.38941800	-2.72815600	0.00000200
H	5.64807700	-1.74640700	0.00000200
H	3.94590400	2.18251300	-0.00000600
H	1.67467200	1.21126200	-0.00000400
O	-1.10962000	-1.81546800	-0.00000400

1' – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-6.80127600	0.42744400	-0.00079100
C	-6.32204300	1.75634900	-0.00001100
C	-4.97318300	2.00354200	0.00052500
C	-4.03379200	0.94213700	0.00030900
C	-4.51903400	-0.41245900	-0.00049700
C	-5.92292100	-0.62474500	-0.00102600
C	-2.63559400	1.19890500	0.00087400
C	-1.82354300	0.11150300	0.00062000
C	-2.26791100	-1.22954300	-0.00018700
C	-3.61234800	-1.50254100	-0.00074600
C	-0.14403500	-1.25067300	0.00043400
N	-1.15221600	-2.06625700	-0.00028800
N	1.15625700	-1.64027600	0.00086000
C	2.34522800	-0.92175500	0.00046800
C	3.53238100	-1.67656600	0.00034300
C	4.76179900	-1.05723600	0.00002600

C	4.82081100	0.33495300	-0.00018300
C	3.65900400	1.09926400	-0.00008200
C	2.42393400	0.47953800	0.00026300
N	6.11189900	0.99505200	-0.00052600
O	6.14175100	2.22466900	-0.00090500
O	7.12513300	0.29768800	-0.00042400
H	-7.86706100	0.24274100	-0.00120200
H	-7.02367300	2.57946400	0.00016400
H	-4.60459500	3.02140600	0.00112500
H	-6.29113900	-1.64270700	-0.00162200
H	-2.25540400	2.21035300	0.00148100
H	-3.98142400	-2.51896400	-0.00135900
H	1.24845500	-2.64562200	0.00073300
H	3.47909400	-2.75657000	0.00045900
H	5.66998200	-1.63826000	-0.00008200
H	3.72422900	2.17564500	-0.00026600
H	1.53319900	1.08164400	0.00037400
O	-0.43789700	0.07795800	0.00105900

1- – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-6.49729500	1.54793800	-0.00002000
C	-6.87199800	0.18697700	-0.00001400
C	-5.90885200	-0.79208000	-0.00001400
C	-4.52992900	-0.46867500	-0.00001900
C	-4.14514500	0.91758700	-0.00002500
C	-5.17044100	1.89906900	-0.00002500
C	-3.53118100	-1.48244600	-0.00001800
C	-2.23305700	-1.07528400	-0.00002400
C	-1.82579400	0.28460500	-0.00002900
C	-2.77362500	1.28059500	-0.00002900
C	-0.03185000	-0.92080900	-0.00002900
C	2.32967700	-0.85474600	-0.00001200
C	3.50121900	-1.66646700	-0.00005600
C	4.76190600	-1.12888100	-0.00003200
C	4.91941600	0.26631400	0.00004000
C	3.79265500	1.09781100	0.00008600
C	2.52759900	0.55725700	0.00006000
N	6.22474400	0.83522400	0.00006900
O	6.34617300	2.07062000	0.00011500
O	7.21050200	0.08072000	0.00003600
H	-7.26047500	2.31487500	-0.00002100
H	-7.91967500	-0.08265400	-0.00001000
H	-6.19510500	-1.83658000	-0.00000900
H	-4.88449800	2.94367100	-0.00003000
H	-3.80786600	-2.52792900	-0.00001400
H	-2.49038500	2.32498900	-0.00003300
H	3.36932400	-2.73958100	-0.00011100
H	5.63388000	-1.76405700	-0.00006800
H	3.92745200	2.16866500	0.00014200
H	1.66641600	1.20371700	0.00009600
O	-1.10574000	-1.83954400	-0.00002500
N	1.14447000	-1.51248100	-0.00003600
N	-0.44441300	0.33553200	-0.00003100

1'- – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-6.74487000	0.48051200	0.09310200
C	-6.25371100	1.77819300	-0.16683200
C	-4.90200600	1.99081400	-0.28593100
C	-3.97521800	0.92841500	-0.15315700
C	-4.47250600	-0.39552400	0.11176100
C	-5.87624200	-0.57350100	0.22766600
C	-2.57410100	1.14801400	-0.27556900
C	-1.76340400	0.06636400	-0.13096000
C	-2.22429500	-1.25078800	0.12846700
C	-3.57492600	-1.48490000	0.25041600
C	-0.06861200	-1.34264500	0.01782000
C	2.29194100	-1.00595400	-0.01631500
C	3.51163600	-1.66331700	-0.35556600
C	4.71977200	-1.01700200	-0.34265100
C	4.77920600	0.33582200	0.02751100
C	3.60569200	1.01317800	0.38549800
C	2.39343100	0.36671300	0.36285800
N	6.02762300	1.01535900	0.04703000
O	6.05895700	2.21457900	0.36958400
O	7.05824800	0.39306900	-0.25919300
H	-7.81065400	0.31878400	0.18597600
H	-6.94439300	2.60413100	-0.27186800
H	-4.52326600	2.98569300	-0.48530800
H	-6.25530400	-1.56820300	0.42709600
H	-2.18668400	2.13783500	-0.47444600
H	-3.95613600	-2.47818100	0.44816300
H	3.45807900	-2.70682800	-0.63298800
H	5.62625900	-1.53600700	-0.61257900
H	3.66437800	2.04878100	0.68336900
H	1.50733400	0.90823700	0.64787100
O	-0.39987000	0.01484200	-0.20015700
N	1.17511200	-1.76755100	-0.03693300
N	-1.13830700	-2.09645500	0.20906300

1t – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-6.38311000	1.64918400	-0.29085800
C	-6.80350600	0.33607900	0.00661700
C	-5.87749400	-0.65953400	0.19508900
C	-4.49025400	-0.39521200	0.09636200
C	-4.06116100	0.94081000	-0.20606100
C	-5.04614700	1.94163600	-0.39399500
C	-3.52841000	-1.42728600	0.29022800
C	-2.22229100	-1.08115500	0.17761500
C	-1.78831700	0.22672200	-0.11688100
C	-2.67547000	1.24417200	-0.31178200
C	0.00436300	-1.13261100	0.11423700
C	2.34095400	-0.98626200	0.09306200
C	3.37458400	-1.48687000	-0.71990000
C	4.60256700	-0.86155100	-0.77192600
C	4.82248000	0.27326200	0.00771500
C	3.82723800	0.77868200	0.84045800
C	2.59739100	0.15214200	0.88235000
N	6.11251500	0.93360400	-0.04166200
O	6.28502700	1.93768600	0.64848800
O	6.98416100	0.46472000	-0.77270000
H	-7.11960800	2.42749900	-0.43794900
H	-7.85929200	0.11537500	0.08579000

H	-6.19845500	-1.66765900	0.42354100
H	-4.72419100	2.94960700	-0.62214000
H	-3.83601600	-2.43826700	0.51559500
H	-2.35209700	2.24995100	-0.53886600
H	3.18874400	-2.37225100	-1.31042500
H	5.38961300	-1.24042700	-1.40443900
H	4.02437700	1.64702300	1.44901900
H	1.83507300	0.52643400	1.55075700
O	-1.11540200	-1.89514400	0.31851700
N	1.14884000	-1.68796900	0.14201300
N	-0.39999500	0.15069900	-0.13545600
H	0.23153200	0.89703600	-0.37358500

1t' – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-6.74617400	0.53320400	-0.03779500
C	-6.23039000	1.82962400	-0.24564300
C	-4.87399800	2.03203100	-0.30201800
C	-3.96792900	0.95429100	-0.15482800
C	-4.49133300	-0.36581000	0.05690800
C	-5.89729400	-0.53495500	0.10923800
C	-2.56059600	1.16283500	-0.21353500
C	-1.77055100	0.07189500	-0.06116900
C	-2.27023800	-1.22969100	0.14720300
C	-3.61185400	-1.47270300	0.20899700
C	-0.01201000	-1.29013500	0.10883000
C	2.33139700	-0.99644800	0.07293000
C	3.47003400	-1.60272100	-0.49408700
C	4.68180900	-0.94787500	-0.54031000
C	4.78235200	0.33306400	0.00169900
C	3.68046000	0.95208800	0.58906700
C	2.46714500	0.29534300	0.62304100
N	6.05203100	1.02708200	-0.03863800
O	6.12022800	2.15917000	0.44129900
O	7.01676000	0.45947700	-0.55218000
H	-7.81639300	0.38280800	0.00530800
H	-6.90769400	2.66490400	-0.36041300
H	-4.47631200	3.02606300	-0.46112300
H	-6.29436800	-1.52916800	0.26881100
H	-2.15086900	2.14973300	-0.37292500
H	-4.00590100	-2.46650500	0.36700700
H	3.37492000	-2.59967300	-0.89951600
H	5.54662800	-1.41441700	-0.98465300
H	3.78308700	1.93774700	1.01486200
H	1.62082200	0.77601600	1.08739300
O	-0.38760600	0.01750500	-0.07792700
N	1.17581600	-1.75292200	0.11037200
N	-1.14627000	-2.03545100	0.24918900
H	-1.12499900	-3.03192900	0.38807900

TS1 – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

1 imaginary frequency – -60.88 cm^{-1}

C	3.45815100	1.06922700	-0.24507800
C	2.30001600	0.32075300	-0.23031400
C	2.35540200	-1.06190900	0.01156600

C	3.60195700	-1.67224500	0.23817200
C	4.75766000	-0.92416500	0.22249700
C	4.68465300	0.44788800	-0.01921500
H	3.41981400	2.13081800	-0.43053400
H	1.35157500	0.80517100	-0.41025100
H	3.65140600	-2.73585600	0.42603900
H	5.71469900	-1.38977500	0.39605200
N	5.89682900	1.23519900	-0.03447000
O	6.97015300	0.66621000	0.16745500
O	5.81062500	2.44483700	-0.24857000
N	1.21684300	-1.84060000	0.01910300
C	-0.07144200	-1.34620200	-0.09848400
N	-0.76831300	-1.21554200	-1.16968500
C	-1.99171800	-0.69210800	-0.73831200
C	-1.93415100	-0.53561500	0.66368100
C	-3.12387900	-0.34779600	-1.43273800
C	-2.95625200	-0.04949300	1.42158100
C	-4.22106400	0.16394300	-0.70175600
H	-3.18465500	-0.46131800	-2.50626200
C	-4.13837000	0.31427400	0.72889700
H	-2.88413500	0.05929600	2.49417300
C	-5.42595800	0.54080300	-1.35439300
C	-5.26327000	0.83210000	1.42317200
C	-6.48898800	1.03624300	-0.64872300
H	-5.48754700	0.42769700	-2.42906600
C	-6.40625300	1.18343100	0.75575600
H	-5.20089700	0.94517900	2.49774500
H	-7.39771400	1.31758500	-1.16320900
H	-7.25274000	1.57609100	1.30263100
H	1.31331300	-2.81942900	0.24335900
O	-0.69072800	-0.95900000	1.06821900

TS2 – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

1 imaginary frequency – -44.45 cm^{-1}

C	3.55612400	1.08044900	-0.18384000
C	2.36824100	0.40124000	-0.16339600
C	2.31962500	-1.01970700	0.02942800
C	3.57729700	-1.68496000	0.19921100
C	4.76089600	-1.00249200	0.17845800
C	4.77214000	0.39359700	-0.01364200
H	3.57201800	2.14977000	-0.32942000
H	1.44233000	0.94392200	-0.29634800
H	3.56743100	-2.75617700	0.34617000
H	5.69702900	-1.52333100	0.30830800
N	5.99328000	1.09753400	-0.03420700
O	7.06106700	0.47222700	0.11960300
O	5.98522500	2.33266000	-0.20575600
N	1.20117400	-1.73772400	0.05530100
C	-0.02151800	-1.22231200	-0.09603700
N	-0.74742400	-1.09445200	-1.17303400
C	-1.98670600	-0.63113500	-0.74347300
C	-1.95274300	-0.49473600	0.66593500
C	-3.12876200	-0.31528200	-1.43600000
C	-3.00178600	-0.06091000	1.41624700
C	-4.25722800	0.14377500	-0.70955300
H	-3.17819500	-0.40956700	-2.51268200

C	-4.19666600	0.27239100	0.72192900
H	-2.94396900	0.03278000	2.49183700
C	-5.46823300	0.48712500	-1.36595800
C	-5.34493900	0.73473500	1.41269400
C	-6.55950900	0.93098200	-0.66371700
H	-5.51612300	0.39144100	-2.44351800
C	-6.49780000	1.05645700	0.74179600
H	-5.29661900	0.83090000	2.49017600
H	-7.47210600	1.18674000	-1.18538400
H	-7.36299500	1.40742700	1.28811700
O	-0.70486700	-0.87072600	1.08188200

TS3 – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

1 imaginary frequency – -83.86 cm^{-1}

C	-3.86817900	1.12051200	0.22377900
C	-2.60069300	0.59492900	0.15101800
C	-2.39712700	-0.78416600	-0.12160700
C	-3.54164500	-1.59789000	-0.31632300
C	-4.80715200	-1.06966200	-0.24338900
C	-4.97939900	0.29328700	0.02743200
H	-4.01432900	2.16925000	0.43059700
H	-1.74395800	1.23682000	0.30115500
H	-3.39980900	-2.64842300	-0.52521600
H	-5.67248900	-1.69606500	-0.39318700
N	-6.29807800	0.84376700	0.10304200
O	-7.26835700	0.09668900	-0.07342600
O	-6.42942500	2.05048700	0.34278900
N	-1.17433300	-1.33671900	-0.20039500
C	0.02320300	-0.92014200	-0.07105600
N	0.81230000	-0.90865200	1.02876900
C	2.10942500	-0.52609200	0.69771200
C	2.07121700	-0.28898200	-0.68930400
C	3.25605200	-0.36595900	1.41968200
C	3.14995500	0.11034100	-1.40947900
C	4.41849000	0.05165100	0.71859300
H	3.29245900	-0.54542800	2.48458500
C	4.36722600	0.29077600	-0.69715900
H	3.09605400	0.28655500	-2.47394300
C	5.65035600	0.24239500	1.39395000
C	5.54776700	0.70686600	-1.36098600
C	6.77290900	0.64588400	0.71780500
H	5.68988700	0.06281800	2.46048200
C	6.72151500	0.88053300	-0.67329200
H	5.50720700	0.88667900	-2.42740300
H	7.70373400	0.78593800	1.25034900
H	7.61305300	1.19854500	-1.19632600
H	0.47571800	-1.17130700	1.94137000
O	0.78649700	-0.52965700	-1.14144100

TS4d – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

1 imaginary frequency – -1969.5 cm^{-1}

C	-3.93298900	1.12041600	-0.00014300
C	-2.63605800	0.65471800	-0.00008500

C	-2.37746100	-0.73269600	0.00000100
C	-3.46517300	-1.62878200	0.00002600
C	-4.76033300	-1.16273200	-0.00003200
C	-4.99363700	0.21383500	-0.00011700
H	-4.13425700	2.17997100	-0.00020900
H	-1.81752300	1.35856900	-0.00010600
H	-3.26684600	-2.69078400	0.00009300
H	-5.59266400	-1.84838200	-0.00001200
N	-6.35030100	0.70632600	-0.00017800
O	-7.27422400	-0.10980200	-0.00015500
O	-6.53622800	1.92503300	-0.00025000
N	-1.11559800	-1.25766600	0.00006500
H	-0.17171100	-2.31571600	0.00019400
C	0.07856600	-0.69122900	0.00004400
N	0.98464400	-1.65627500	0.00016100
C	2.22693700	-1.03590900	0.00013600
C	1.96031200	0.36267900	0.00000100
C	3.51900400	-1.48625500	0.00021100
C	2.91336100	1.32321600	-0.00006300
C	4.56434600	-0.52527300	0.00014800
H	3.74853900	-2.54225700	0.00031300
C	4.26653200	0.88039500	0.00001100
H	2.67152900	2.37630600	-0.00016700
C	5.92535000	-0.92471900	0.00021600
C	5.33695900	1.80699600	-0.00004800
C	6.93700500	0.00133400	0.00015400
H	6.15422300	-1.98264000	0.00031800
C	6.64135800	1.38136100	0.00002100
H	5.10744800	2.86471700	-0.00015100
H	7.96817900	-0.32515100	0.00020800
H	7.44674500	2.10305500	-0.00002700
O	0.56428200	0.55120500	-0.00005400

TS4w – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

1 imaginary frequency – -991.28 cm^{-1}

C	-3.61101000	-1.57701300	0.27036800
C	-2.39009400	-0.92831200	0.28324500
C	-2.32304700	0.44762600	0.01446400
C	-3.50957400	1.15142300	-0.25717700
C	-4.72684000	0.50463600	-0.26936900
C	-4.77015100	-0.86182100	-0.00676800
H	-3.66728700	-2.63335500	0.47949500
H	-1.50284900	-1.49234400	0.50947800
H	-3.45808200	2.21041000	-0.46304600
H	-5.63537500	1.04471300	-0.48240500
N	-6.05001600	-1.55197200	-0.01821700
O	-7.06305700	-0.89819400	-0.25580600
O	-6.06510500	-2.75935800	0.21019600
N	-1.15147100	1.20953400	0.02078600
C	0.10242600	0.79451100	0.02810000
N	1.17596400	1.58176700	0.05089100
C	2.30181700	0.76134200	0.02286000
C	1.82591000	-0.56105700	-0.01314100
C	3.64372900	1.02381700	0.02483800
C	2.61825400	-1.66032000	-0.04722200
C	4.53054700	-0.08390500	-0.01016300

H	4.02934200	2.03270700	0.05096800
C	4.02095300	-1.42774300	-0.04634600
H	2.21775300	-2.66303400	-0.07519700
C	5.93637100	0.10556700	-0.01126200
C	4.93958000	-2.50588500	-0.08115400
C	6.79488000	-0.96250100	-0.04572000
H	6.32254000	1.11620300	0.01559700
C	6.29229300	-2.28162800	-0.08095600
H	4.55255500	-3.51619700	-0.10825300
H	7.86365400	-0.79702100	-0.04615600
H	6.97933000	-3.11632400	-0.10799800
H	1.15930000	2.70709100	0.07384100
O	0.99358100	4.12163600	0.02857200
H	-0.18882000	4.05800000	0.04092500
H	1.29072900	4.53851200	0.84273000
O	-1.38938000	3.76617700	-0.03726200
H	-1.84526400	4.10854700	0.73726300
H	-1.28735100	2.32212000	0.01204300
O	0.43548900	-0.50873100	-0.00833600

MC1' – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	-3.59745700	-1.36613900	0.77242000
C	-2.41540100	-0.65405300	0.74911900
C	-2.29164800	0.50921100	-0.03517400
C	-3.40624200	0.93672900	-0.77948200
C	-4.58824200	0.22581700	-0.76674800
C	-4.67779500	-0.92730000	0.00992400
H	-3.69279500	-2.25303300	1.37864600
H	-1.58552300	-0.98859300	1.35172400
H	-3.32331000	1.83253400	-1.37758000
H	-5.43591400	0.55156500	-1.34834500
N	-5.91751200	-1.67868100	0.03082500
O	-6.86504700	-1.26643000	-0.63758600
O	-5.97436700	-2.69978900	0.71538300
N	-1.15804200	1.31288800	-0.05850500
C	0.04134500	0.85303200	-0.02148800
N	1.17912100	1.58632200	0.07472300
C	2.28180300	0.74489800	0.02906400
C	1.75874200	-0.55694200	-0.09812900
C	3.62919900	0.96229300	0.08190900
C	2.52413800	-1.67304600	-0.17713300
C	4.48512300	-0.17011100	0.00478400
H	4.04501000	1.95492300	0.17912700
C	3.93508400	-1.49023000	-0.12554200
H	2.09414500	-2.65933900	-0.27517700
C	5.89448700	-0.02750400	0.05296000
C	4.81911800	-2.59361100	-0.20060900
C	6.72128000	-1.11995800	-0.02264600
H	6.31167800	0.96646300	0.15122900
C	6.17913600	-2.41619500	-0.15074000
H	4.40114200	-3.58722000	-0.29871400
H	7.79428000	-0.98935300	0.01592800
H	6.83922600	-3.27086100	-0.20953100
H	1.19806200	2.61101800	0.16675500
O	1.13635200	4.40379900	0.39584900
H	1.54117500	4.92260900	-0.30616800
H	0.16616500	4.51072300	0.29126400

O	-1.58536700	4.13058900	0.21532900
H	-2.04238700	4.48950100	-0.55165700
H	-1.50771200	3.16184800	0.06026400
O	0.37790000	-0.47039800	-0.12547600

MC1t' – cartesian coordinates optimized structure B3LYP/6-311++G(2df,2p)/PCM(DMSO)

C	3.61743100	-1.63883900	0.01835100
C	2.38989300	-1.00426300	0.03158100
C	2.32467400	0.39860000	0.01497000
C	3.52268600	1.13804000	-0.01523400
C	4.74452700	0.50380900	-0.02754400
C	4.78806700	-0.88889600	-0.01051800
H	3.66980100	-2.71587400	0.03144100
H	1.49465900	-1.59848300	0.05560000
H	3.47889900	2.21716600	-0.03410400
H	5.65928500	1.07402200	-0.05199700
N	6.07074700	-1.56445100	-0.02376500
O	7.09247300	-0.87960700	-0.04651300
O	6.08633800	-2.79450900	-0.01160800
N	1.14841800	1.14057700	0.02801600
C	-0.14446200	0.75174400	0.01921200
N	-1.16999200	1.55823500	0.00387900
C	-2.28294000	0.71797500	0.00309000
C	-1.82838200	-0.61748700	0.01696600
C	-3.62845300	0.98336000	-0.00934900
C	-2.63262800	-1.71053700	0.01908900
C	-4.52738900	-0.11332100	-0.00730100
H	-4.00571700	1.99658200	-0.02072900
C	-4.03258600	-1.46412700	0.00692000
H	-2.24457100	-2.71887100	0.02959500
C	-5.93246700	0.08930300	-0.01911300
C	-4.96417100	-2.53227300	0.00855300
C	-6.80321700	-0.96922200	-0.01704600
H	-6.30787000	1.10455200	-0.02990100
C	-6.31467900	-2.29457600	-0.00311000
H	-4.58833400	-3.54738200	0.01916300
H	-7.87022900	-0.79211600	-0.02619100
H	-7.01049300	-3.12258400	-0.00173000
H	-1.27310400	3.40131300	-0.09667300
O	-1.17405100	4.37556200	-0.20595000
H	-1.65206000	4.77750400	0.52597100
H	0.60392000	4.31659200	0.00366900
O	1.53339000	4.00256300	0.04466500
H	1.90095000	4.37044000	0.85442100
H	1.27052300	2.16171100	0.04359700
O	-0.44381400	-0.57411300	0.02738800

Annex II: Excitation energies, oscillator strengths, spin and spatial symmetry, the S^2 and the largest coefficients in the CI expansion for all TD-DFT vertical excitation energies computed

Single-point TDDFT B3LYP/6-311++G(2df,2p)/PCM(DMSO) over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometry

1

Excited State 1: Singlet-A 2.7439 eV 451.86 nm f=0.2127 <S**2>=0.000
79 -> 80 0.70591
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.54577425
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1476 eV 393.90 nm f=0.4555 <S**2>=0.000
78 -> 80 0.70313

Excited State 3: Singlet-A 3.8331 eV 323.46 nm f=0.0000 <S**2>=0.000
73 -> 80 -0.20422
74 -> 80 0.66463

Excited State 4: Singlet-A 3.9789 eV 311.60 nm f=0.3330 <S**2>=0.000
77 -> 80 -0.41852
79 -> 81 0.54725

Excited State 5: Singlet-A 4.0729 eV 304.41 nm f=0.1309 <S**2>=0.000
76 -> 80 0.10771
77 -> 80 0.54626
79 -> 81 0.40135
79 -> 83 0.10052

Excited State 6: Singlet-A 4.1382 eV 299.61 nm f=0.0078 <S**2>=0.000
76 -> 80 0.65573
78 -> 82 -0.11858
79 -> 82 -0.13816

Excited State 7: Singlet-A 4.1965 eV 295.45 nm f=0.0418 <S**2>=0.000
78 -> 81 0.58930
79 -> 81 -0.10635
79 -> 82 0.10519
79 -> 83 0.31370
79 -> 84 -0.12441

Excited State 8: Singlet-A 4.4621 eV 277.86 nm f=0.0004 <S**2>=0.000
70 -> 80 0.67016
73 -> 80 0.17915

Excited State 9: Singlet-A 4.4862 eV 276.37 nm f=0.0475 <S**2>=0.000
76 -> 80 0.16664
78 -> 81 -0.10368
78 -> 82 0.11936
79 -> 82 0.66243

Excited State 10: Singlet-A 4.7214 eV 262.60 nm f=0.0040 <S**2>=0.000
75 -> 80 0.69180

Excited State 11: Singlet-A 4.8282 eV 256.79 nm f=0.6326 <S**2>=0.000
77 -> 81 -0.22713
78 -> 81 -0.29906
78 -> 82 0.20760
78 -> 84 0.12025
79 -> 83 0.52219

Excited State 12: Singlet-A 4.8962 eV 253.22 nm f=0.2115 <S**2>=0.000
78 -> 81 0.10153
78 -> 82 0.63693
79 -> 82 -0.13308

79 -> 83 -0.16752

Excited State 13: Singlet-A 4.9977 eV 248.08 nm f=0.0002 <S**2>=0.000
70 -> 80 -0.18302
73 -> 80 0.64383
74 -> 80 0.19940

Excited State 14: Singlet-A 5.1172 eV 242.29 nm f=0.0032 <S**2>=0.000
75 -> 81 -0.12426
77 -> 81 0.33149
79 -> 83 0.16165
79 -> 84 0.53291
79 -> 87 -0.20301

Excited State 15: Singlet-A 5.1754 eV 239.57 nm f=0.0000 <S**2>=0.000
79 -> 85 0.63734
79 -> 86 -0.25187
79 -> 89 0.12045

Excited State 16: Singlet-A 5.2617 eV 235.64 nm f=0.0500 <S**2>=0.000
75 -> 81 0.12854
77 -> 81 0.33497
78 -> 83 0.40724
79 -> 83 0.12801
79 -> 87 0.40234

Excited State 17: Singlet-A 5.3366 eV 232.33 nm f=0.0179 <S**2>=0.000
72 -> 80 -0.10741
75 -> 81 0.10975
78 -> 83 -0.38619
79 -> 84 0.27448
79 -> 87 0.47510

Excited State 18: Singlet-A 5.3810 eV 230.41 nm f=0.0006 <S**2>=0.000
78 -> 85 0.21223
79 -> 85 0.21020
79 -> 86 0.61093
79 -> 88 0.10703
79 -> 89 0.11133

Excited State 19: Singlet-A 5.4592 eV 227.11 nm f=0.0173 <S**2>=0.000
72 -> 80 0.67698

Excited State 20: Singlet-A 5.5699 eV 222.60 nm f=0.0281 <S**2>=0.000
75 -> 83 0.12135
78 -> 84 0.61346
78 -> 87 -0.23727

Excited State 21: Singlet-A 5.5874 eV 221.90 nm f=0.0002 <S**2>=0.000
78 -> 85 -0.31900
79 -> 88 0.57352
79 -> 89 -0.14339
79 -> 90 0.17194

Excited State 22: Singlet-A 5.6115 eV 220.95 nm f=0.0011 <S**2>=0.000
78 -> 85 0.54387
78 -> 89 0.10436
79 -> 86 -0.17685
79 -> 88 0.25314

79 -> 89 -0.26223

Excited State 23: Singlet-A 5.6418 eV 219.76 nm f=0.2595 <S**2>=0.000
76 -> 81 0.20779
76 -> 84 -0.11577
77 -> 81 -0.22794
77 -> 82 0.48878
78 -> 83 0.23019
79 -> 84 0.15709

Excited State 24: Singlet-A 5.7188 eV 216.80 nm f=0.4391 <S**2>=0.000
76 -> 81 0.37690
77 -> 81 0.32149
77 -> 82 0.23518
78 -> 83 -0.26685
79 -> 83 0.12467
79 -> 84 -0.21718
79 -> 87 -0.10500

Excited State 25: Singlet-A 5.7300 eV 216.38 nm f=0.0007 <S**2>=0.000
78 -> 86 -0.30869
79 -> 85 -0.14900
79 -> 86 -0.13140
79 -> 88 0.19515
79 -> 89 0.53613

Excited State 26: Singlet-A 5.7628 eV 215.15 nm f=0.1601 <S**2>=0.000
75 -> 81 -0.21983
75 -> 83 -0.10047
78 -> 83 -0.10213
78 -> 84 0.25354
78 -> 87 0.55391
79 -> 84 -0.10879

Excited State 27: Singlet-A 5.8316 eV 212.61 nm f=0.0035 <S**2>=0.000
78 -> 86 0.48810
78 -> 88 0.20402
79 -> 85 -0.10986
79 -> 88 0.16557
79 -> 89 0.21260
79 -> 90 -0.33687

Excited State 28: Singlet-A 5.8627 eV 211.48 nm f=0.0399 <S**2>=0.000
71 -> 80 0.24533
75 -> 81 0.22984
76 -> 81 0.45665
77 -> 82 -0.26592
78 -> 87 0.19714
79 -> 84 0.11253

Excited State 29: Singlet-A 5.8731 eV 211.10 nm f=0.0003 <S**2>=0.000
78 -> 85 0.10471
78 -> 86 0.35913
78 -> 88 -0.14621
79 -> 89 0.14323
79 -> 90 0.52653

Excited State 30: Singlet-A 5.9114 eV 209.74 nm f=0.0131 <S**2>=0.000
71 -> 80 -0.23532

75 -> 81 0.54652
76 -> 81 -0.19474
77 -> 82 0.12799
78 -> 87 0.18302
79 -> 87 -0.13311

1-

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4794 eV 500.05 nm f=0.9453 <S**2>=0.000
79 -> 80 0.70408
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.08769575
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9943 eV 414.06 nm f=0.2121 <S**2>=0.000
78 -> 80 0.69836

Excited State 3: Singlet-A 3.5872 eV 345.63 nm f=0.2603 <S**2>=0.000
77 -> 80 -0.23937
79 -> 81 0.64959

Excited State 4: Singlet-A 3.7474 eV 330.86 nm f=0.0000 <S**2>=0.000
72 -> 80 0.57737
73 -> 80 -0.17584
76 -> 80 -0.34679

Excited State 5: Singlet-A 3.8649 eV 320.80 nm f=0.0711 <S**2>=0.000
77 -> 80 0.63566
78 -> 83 -0.10462
79 -> 81 0.20403
79 -> 83 0.15943

Excited State 6: Singlet-A 3.9968 eV 310.21 nm f=0.0001 <S**2>=0.000
72 -> 80 0.33278
76 -> 80 0.60937

Excited State 7: Singlet-A 4.0030 eV 309.73 nm f=0.0050 <S**2>=0.000
75 -> 80 0.53477
79 -> 82 -0.44044

Excited State 8: Singlet-A 4.1117 eV 301.54 nm f=0.0034 <S**2>=0.000
75 -> 80 0.34933
78 -> 81 0.41723
79 -> 82 0.38519
79 -> 83 0.17238

Excited State 9: Singlet-A 4.1687 eV 297.42 nm f=0.0692 <S**2>=0.000
75 -> 80 -0.27638
78 -> 81 0.43201
79 -> 82 -0.37247
79 -> 83 0.28100

Excited State 10: Singlet-A 4.4833 eV 276.55 nm f=0.0000 <S**2>=0.000
69 -> 80 0.52023
72 -> 80 -0.13481
73 -> 80 -0.44276

Excited State 11: Singlet-A 4.4876 eV 276.28 nm f=0.3950 <S**2>=0.000

77 -> 80 -0.12812
77 -> 81 -0.11024
78 -> 81 -0.32314
79 -> 83 0.56615
79 -> 86 0.13584

Excited State 12: Singlet-A 4.5253 eV 273.98 nm f=0.0007 <S**2>=0.000
79 -> 84 0.66256
79 -> 85 0.17931
79 -> 89 -0.12522

Excited State 13: Singlet-A 4.6103 eV 268.93 nm f=0.0007 <S**2>=0.000
69 -> 80 0.45688
72 -> 80 0.13980
73 -> 80 0.50694

Excited State 14: Singlet-A 4.6860 eV 264.58 nm f=0.0043 <S**2>=0.000
74 -> 80 0.51785
79 -> 86 0.44323

Excited State 15: Singlet-A 4.7472 eV 261.17 nm f=0.0046 <S**2>=0.000
78 -> 84 0.12322
79 -> 84 -0.16322
79 -> 85 0.66312

Excited State 16: Singlet-A 4.7821 eV 259.27 nm f=0.0334 <S**2>=0.000
77 -> 81 0.44394
78 -> 82 0.27293
78 -> 83 0.37602
79 -> 83 0.17143
79 -> 86 -0.11713
79 -> 88 0.11242

Excited State 17: Singlet-A 4.8041 eV 258.08 nm f=0.0202 <S**2>=0.000
74 -> 80 -0.46417
77 -> 81 0.15766
79 -> 86 0.46938
79 -> 88 -0.13918

Excited State 18: Singlet-A 4.9630 eV 249.82 nm f=0.0009 <S**2>=0.000
79 -> 87 0.68315
79 -> 90 0.11614

Excited State 19: Singlet-A 4.9762 eV 249.15 nm f=0.0912 <S**2>=0.000
77 -> 81 -0.14729
78 -> 82 0.59970
78 -> 83 -0.16393
79 -> 88 -0.27070

Excited State 20: Singlet-A 5.0019 eV 247.88 nm f=0.0307 <S**2>=0.000
71 -> 80 -0.12878
78 -> 82 0.19904
78 -> 83 -0.24169
78 -> 86 0.13047
79 -> 86 0.12866
79 -> 88 0.57181

Excited State 21: Singlet-A 5.0232 eV 246.82 nm f=0.0002 <S**2>=0.000
78 -> 85 0.10793

79 -> 84 0.13794
79 -> 89 0.67020

Excited State 22: Singlet-A 5.1424 eV 241.10 nm f=0.0007 <S**2>=0.000
78 -> 84 0.62888
78 -> 85 -0.23426
78 -> 89 -0.10615
79 -> 85 -0.11039

Excited State 23: Singlet-A 5.2174 eV 237.64 nm f=0.0000 <S**2>=0.000
78 -> 87 0.12158
79 -> 87 -0.11290
79 -> 90 0.67858

Excited State 24: Singlet-A 5.2324 eV 236.96 nm f=0.0248 <S**2>=0.000
71 -> 80 0.45975
77 -> 81 0.12067
78 -> 83 -0.20331
78 -> 86 -0.42037
78 -> 88 0.14086
79 -> 88 0.12599

Excited State 25: Singlet-A 5.2720 eV 235.18 nm f=0.0349 <S**2>=0.000
71 -> 80 0.47334
77 -> 81 0.11452
78 -> 86 0.47149
78 -> 88 -0.10063

Excited State 26: Singlet-A 5.3845 eV 230.26 nm f=0.0002 <S**2>=0.000
76 -> 81 0.68562

Excited State 27: Singlet-A 5.4057 eV 229.36 nm f=0.0003 <S**2>=0.000
78 -> 84 0.17415
78 -> 85 0.59583
78 -> 89 -0.26645
79 -> 91 0.13155

Excited State 28: Singlet-A 5.5229 eV 224.49 nm f=0.0002 <S**2>=0.000
78 -> 87 0.38855
79 -> 91 0.53986
79 -> 93 -0.10784

Excited State 29: Singlet-A 5.5315 eV 224.14 nm f=0.8054 <S**2>=0.000
71 -> 80 0.15241
74 -> 81 -0.10951
77 -> 81 -0.40189
77 -> 82 0.17711
78 -> 83 0.40871
78 -> 88 0.10657
79 -> 86 0.10167
79 -> 88 0.17440

Excited State 30: Singlet-A 5.5333 eV 224.07 nm f=0.0000 <S**2>=0.000
78 -> 84 0.13242
78 -> 85 0.13363
78 -> 87 0.53399
78 -> 89 0.11938
78 -> 90 -0.10435
79 -> 91 -0.35711

1’

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7029 eV 458.71 nm f=0.3553 <S**2>=0.000
79 -> 80 0.70630
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.54483808
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1616 eV 392.16 nm f=0.3653 <S**2>=0.000
78 -> 80 0.70259

Excited State 3: Singlet-A 3.8304 eV 323.68 nm f=0.0000 <S**2>=0.000
74 -> 80 0.69461

Excited State 4: Singlet-A 3.9217 eV 316.15 nm f=0.3669 <S**2>=0.000
77 -> 80 -0.26327
79 -> 81 0.63405

Excited State 5: Singlet-A 4.0458 eV 306.45 nm f=0.0811 <S**2>=0.000
77 -> 80 0.63822
79 -> 81 0.24493
79 -> 83 0.10893

Excited State 6: Singlet-A 4.1489 eV 298.84 nm f=0.0071 <S**2>=0.000
76 -> 80 0.64011
78 -> 82 0.12191
79 -> 82 0.22133

Excited State 7: Singlet-A 4.2164 eV 294.05 nm f=0.0266 <S**2>=0.000
78 -> 81 0.58080
79 -> 81 -0.10785
79 -> 83 0.33270
79 -> 84 -0.13551

Excited State 8: Singlet-A 4.4148 eV 280.84 nm f=0.0179 <S**2>=0.000
76 -> 80 -0.24065
79 -> 82 0.65312

Excited State 9: Singlet-A 4.4689 eV 277.44 nm f=0.0004 <S**2>=0.000
70 -> 80 0.69454

Excited State 10: Singlet-A 4.7364 eV 261.77 nm f=0.0032 <S**2>=0.000
75 -> 80 0.69615

Excited State 11: Singlet-A 4.7696 eV 259.95 nm f=0.6956 <S**2>=0.000
77 -> 81 -0.20657
78 -> 81 -0.34122
78 -> 82 0.15492
78 -> 84 0.10902
79 -> 83 0.52724

Excited State 12: Singlet-A 4.8996 eV 253.05 nm f=0.0804 <S**2>=0.000
78 -> 82 0.65074
79 -> 82 -0.10496
79 -> 83 -0.16388
79 -> 84 -0.11878

Excited State 13: Singlet-A 5.0675 eV 244.66 nm f=0.0052 <S**2>=0.000
75 -> 81 -0.10752
77 -> 81 0.38253
78 -> 82 0.11977
79 -> 83 0.15287
79 -> 84 0.49662
79 -> 87 -0.16675

Excited State 14: Singlet-A 5.0882 eV 243.67 nm f=0.0003 <S**2>=0.000
79 -> 85 0.66209
79 -> 86 -0.15558
79 -> 88 -0.10274
79 -> 89 0.11097

Excited State 15: Singlet-A 5.1474 eV 240.87 nm f=0.0002 <S**2>=0.000
73 -> 80 0.69733

Excited State 16: Singlet-A 5.2189 eV 237.57 nm f=0.0216 <S**2>=0.000
75 -> 81 0.12182
77 -> 81 0.30779
78 -> 83 0.35610
79 -> 83 0.11418
79 -> 84 -0.11988
79 -> 87 0.46466

Excited State 17: Singlet-A 5.3054 eV 233.69 nm f=0.0347 <S**2>=0.000
72 -> 80 -0.10144
77 -> 81 -0.12323
78 -> 83 -0.40984
79 -> 84 0.28992
79 -> 87 0.44259

Excited State 18: Singlet-A 5.3120 eV 233.40 nm f=0.0011 <S**2>=0.000
78 -> 85 0.16897
79 -> 85 0.12341
79 -> 86 0.65426

Excited State 19: Singlet-A 5.4644 eV 226.89 nm f=0.0168 <S**2>=0.000
72 -> 80 0.67604
77 -> 81 0.10080
78 -> 83 -0.11730

Excited State 20: Singlet-A 5.5412 eV 223.75 nm f=0.0000 <S**2>=0.000
79 -> 85 0.10109
79 -> 88 0.65729
79 -> 89 0.10176
79 -> 90 -0.18440

Excited State 21: Singlet-A 5.5809 eV 222.16 nm f=0.0423 <S**2>=0.000
75 -> 83 0.12305
77 -> 83 -0.12723
78 -> 84 0.59168
78 -> 87 -0.23333
79 -> 84 0.13069

Excited State 22: Singlet-A 5.6131 eV 220.88 nm f=0.0003 <S**2>=0.000
78 -> 85 0.62032
78 -> 89 0.11863

79 -> 86 -0.13798
79 -> 89 -0.22901

Excited State 23: Singlet-A 5.6300 eV 220.22 nm f=0.2358 <S**2>=0.000
76 -> 81 -0.21273
76 -> 83 0.10080
76 -> 84 0.10690
77 -> 81 -0.21603
77 -> 82 0.50728
78 -> 83 0.20924
79 -> 84 0.16222

Excited State 24: Singlet-A 5.6984 eV 217.58 nm f=0.0010 <S**2>=0.000
78 -> 85 0.18334
78 -> 86 -0.24025
79 -> 85 -0.13289
79 -> 86 -0.10778
79 -> 89 0.58897

Excited State 25: Singlet-A 5.7269 eV 216.49 nm f=0.5222 <S**2>=0.000
76 -> 81 0.32900
77 -> 81 -0.32122
77 -> 82 -0.23438
78 -> 83 0.30178
78 -> 87 0.15203
79 -> 84 0.22178

Excited State 26: Singlet-A 5.7797 eV 214.52 nm f=0.1517 <S**2>=0.000
75 -> 81 -0.30697
78 -> 84 0.27323
78 -> 87 0.50972
79 -> 87 0.11289

Excited State 27: Singlet-A 5.7899 eV 214.14 nm f=0.0011 <S**2>=0.000
78 -> 86 -0.15331
78 -> 88 0.17888
79 -> 88 0.17972
79 -> 90 0.61768

Excited State 28: Singlet-A 5.8674 eV 211.31 nm f=0.0043 <S**2>=0.000
78 -> 85 0.12667
78 -> 86 0.61873
79 -> 89 0.18066
79 -> 90 0.17571

Excited State 29: Singlet-A 5.8771 eV 210.96 nm f=0.0612 <S**2>=0.000
71 -> 80 -0.35353
76 -> 81 0.50319
77 -> 82 0.25772
78 -> 83 -0.10805

Excited State 30: Singlet-A 5.9291 eV 209.11 nm f=0.0083 <S**2>=0.000
75 -> 81 0.56187
78 -> 87 0.32875
79 -> 87 -0.10738
79 -> 92 0.13330

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4553 eV 504.96 nm f=0.9945 <S**2>=0.000
79 -> 80 0.70435
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.08571915
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0222 eV 410.24 nm f=0.1404 <S**2>=0.000
78 -> 80 0.69440
79 -> 81 -0.11552

Excited State 3: Singlet-A 3.5098 eV 353.25 nm f=0.2743 <S**2>=0.000
77 -> 80 0.36539
79 -> 81 0.58454

Excited State 4: Singlet-A 3.7018 eV 334.93 nm f=0.0310 <S**2>=0.000
72 -> 80 0.26110
74 -> 80 0.11183
75 -> 80 -0.10535
76 -> 80 -0.19629
77 -> 80 0.47665
79 -> 81 -0.32444
79 -> 83 0.11013

Excited State 5: Singlet-A 3.7866 eV 327.43 nm f=0.0141 <S**2>=0.000
72 -> 80 0.57838
74 -> 80 0.13034
76 -> 80 -0.11130
77 -> 80 -0.30097
79 -> 81 0.11814

Excited State 6: Singlet-A 3.9899 eV 310.75 nm f=0.0006 <S**2>=0.000
75 -> 80 0.30336
76 -> 80 -0.19870
79 -> 82 0.59536

Excited State 7: Singlet-A 4.1031 eV 302.17 nm f=0.0236 <S**2>=0.000
72 -> 80 0.12319
75 -> 80 -0.15582
76 -> 80 0.41465
78 -> 81 0.30502
79 -> 82 0.22017
79 -> 83 0.35225

Excited State 8: Singlet-A 4.1363 eV 299.75 nm f=0.0201 <S**2>=0.000
75 -> 80 0.44901
76 -> 80 -0.17102
78 -> 81 0.32006
79 -> 82 -0.28374
79 -> 83 0.25887

Excited State 9: Singlet-A 4.1981 eV 295.33 nm f=0.0034 <S**2>=0.000
72 -> 80 0.19998
75 -> 80 0.38374
76 -> 80 0.40360
77 -> 80 0.14310
78 -> 81 -0.31540

Excited State 10: Singlet-A 4.4189 eV 280.58 nm f=0.2642 <S**2>=0.000
76 -> 80 -0.10638
77 -> 80 -0.10492
78 -> 81 -0.33551
79 -> 83 0.42498
79 -> 84 0.36450
79 -> 85 0.13148

Excited State 11: Singlet-A 4.4690 eV 277.43 nm f=0.1293 <S**2>=0.000
78 -> 81 0.22253
79 -> 83 -0.25099
79 -> 84 0.56844
79 -> 86 0.14027

Excited State 12: Singlet-A 4.5300 eV 273.70 nm f=0.0005 <S**2>=0.000
69 -> 80 0.69210

Excited State 13: Singlet-A 4.6645 eV 265.80 nm f=0.0204 <S**2>=0.000
74 -> 80 0.27806
77 -> 81 0.21201
78 -> 81 -0.14125
79 -> 85 -0.38010
79 -> 86 0.41578

Excited State 14: Singlet-A 4.6928 eV 264.20 nm f=0.0043 <S**2>=0.000
78 -> 84 -0.10723
79 -> 84 -0.10153
79 -> 85 0.51964
79 -> 86 0.41640

Excited State 15: Singlet-A 4.7037 eV 263.59 nm f=0.0005 <S**2>=0.000
73 -> 80 0.68590

Excited State 16: Singlet-A 4.7395 eV 261.60 nm f=0.0072 <S**2>=0.000
77 -> 81 0.49272
78 -> 83 0.34566
79 -> 83 -0.14739
79 -> 85 0.12273
79 -> 87 0.19469
79 -> 88 0.14757

Excited State 17: Singlet-A 4.8226 eV 257.09 nm f=0.0004 <S**2>=0.000
72 -> 80 -0.10733
74 -> 80 0.57684
76 -> 80 0.10787
79 -> 86 -0.20522
79 -> 87 0.21142
79 -> 88 0.13385

Excited State 18: Singlet-A 4.8917 eV 253.46 nm f=0.0085 <S**2>=0.000
74 -> 80 -0.12306
78 -> 83 -0.12450
79 -> 86 0.10246
79 -> 87 0.57375
79 -> 88 -0.23328
79 -> 89 0.14688

Excited State 19: Singlet-A 4.9481 eV 250.57 nm f=0.0419 <S**2>=0.000
74 -> 80 -0.10755

78 -> 82 -0.36322
78 -> 83 -0.15110
79 -> 87 0.12003
79 -> 88 0.48512
79 -> 89 -0.19257

Excited State 20: Singlet-A 4.9654 eV 249.70 nm f=0.0215 <S**2>=0.000
78 -> 82 0.56614
78 -> 83 -0.12022
79 -> 86 0.11938
79 -> 87 0.15924
79 -> 88 0.18330
79 -> 89 -0.22968

Excited State 21: Singlet-A 4.9960 eV 248.17 nm f=0.0219 <S**2>=0.000
78 -> 82 0.11983
78 -> 83 -0.12452
79 -> 87 -0.10011
79 -> 88 0.27873
79 -> 89 0.58283

Excited State 22: Singlet-A 5.1605 eV 240.26 nm f=0.0022 <S**2>=0.000
79 -> 90 0.67601

Excited State 23: Singlet-A 5.1763 eV 239.52 nm f=0.0065 <S**2>=0.000
78 -> 84 0.63468
78 -> 85 -0.18042
78 -> 89 -0.11352

Excited State 24: Singlet-A 5.2310 eV 237.02 nm f=0.3712 <S**2>=0.000
71 -> 80 0.36290
75 -> 81 -0.13860
76 -> 81 -0.26898
77 -> 81 0.30549
78 -> 83 -0.35211

Excited State 25: Singlet-A 5.2885 eV 234.44 nm f=0.0178 <S**2>=0.000
74 -> 81 0.11456
76 -> 81 0.16979
78 -> 85 -0.36026
78 -> 86 0.50337
78 -> 87 -0.10361
78 -> 88 -0.10632

Excited State 26: Singlet-A 5.3438 eV 232.02 nm f=0.0632 <S**2>=0.000
71 -> 80 0.56137
75 -> 81 0.11144
76 -> 81 0.24461
77 -> 81 -0.10727
77 -> 82 -0.10070
78 -> 83 0.14134
79 -> 88 0.11598

Excited State 27: Singlet-A 5.4175 eV 228.86 nm f=0.0004 <S**2>=0.000
78 -> 84 0.13061
78 -> 85 0.46109
78 -> 86 0.35329
78 -> 89 -0.22470
79 -> 91 0.25097

Excited State 28: Singlet-A 5.4677 eV 226.76 nm f=0.0050 <S**2>=0.000
75 -> 81 0.21011
76 -> 82 -0.16093
77 -> 82 0.60794

Excited State 29: Singlet-A 5.4744 eV 226.48 nm f=0.0094 <S**2>=0.000
78 -> 84 -0.13123
78 -> 85 -0.20362
78 -> 86 -0.13393
79 -> 91 0.59965

Excited State 30: Singlet-A 5.5600 eV 222.99 nm f=0.0484 <S**2>=0.000
76 -> 81 0.15913
78 -> 83 -0.11869
78 -> 87 0.41634
79 -> 91 0.14171
79 -> 92 -0.40329
79 -> 93 -0.15485
79 -> 94 0.20290

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8608 eV 433.39 nm f=0.3286 <S**2>=0.000
79 -> 80 0.69861
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.53498016
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1037 eV 399.47 nm f=0.1742 <S**2>=0.000
78 -> 80 0.69884

Excited State 3: Singlet-A 3.7911 eV 327.04 nm f=0.2966 <S**2>=0.000
73 -> 80 0.35306
74 -> 80 0.12696
75 -> 80 -0.13108
77 -> 80 0.55390
79 -> 81 0.14182

Excited State 4: Singlet-A 3.8413 eV 322.77 nm f=0.1159 <S**2>=0.000
73 -> 80 0.55313
74 -> 80 0.12705
77 -> 80 -0.37859

Excited State 5: Singlet-A 4.0680 eV 304.78 nm f=0.1362 <S**2>=0.000
76 -> 80 0.26478
77 -> 80 -0.14960
78 -> 81 0.18147
78 -> 83 -0.16784
79 -> 81 0.55694
79 -> 83 0.13183

Excited State 6: Singlet-A 4.0897 eV 303.16 nm f=0.0456 <S**2>=0.000
76 -> 80 0.62471
77 -> 80 0.10535
79 -> 81 -0.22139
79 -> 82 -0.11795

Excited State 7: Singlet-A 4.2520 eV 291.59 nm f=0.0558 <S**2>=0.000
78 -> 81 0.60810
79 -> 81 -0.25877
79 -> 83 0.21930

Excited State 8: Singlet-A 4.4725 eV 277.22 nm f=0.0005 <S**2>=0.000
71 -> 80 0.69160

Excited State 9: Singlet-A 4.5698 eV 271.31 nm f=0.0114 <S**2>=0.000
76 -> 80 0.14840
78 -> 82 0.21525
79 -> 82 0.64386

Excited State 10: Singlet-A 4.6687 eV 265.57 nm f=0.0301 <S**2>=0.000
73 -> 80 0.19109
74 -> 80 -0.21444
75 -> 80 0.60635
79 -> 83 -0.10352

Excited State 11: Singlet-A 4.8051 eV 258.02 nm f=0.3891 <S**2>=0.000
75 -> 80 -0.11667
77 -> 81 0.44181
78 -> 81 0.21185
78 -> 83 0.16502
78 -> 84 0.14035
79 -> 81 0.10824
79 -> 83 -0.39294

Excited State 12: Singlet-A 4.9182 eV 252.09 nm f=0.0024 <S**2>=0.000
74 -> 80 -0.13358
78 -> 82 0.64145
79 -> 82 -0.22967

Excited State 13: Singlet-A 4.9323 eV 251.37 nm f=0.0027 <S**2>=0.000
73 -> 80 -0.10366
74 -> 80 0.61682
75 -> 80 0.26271
78 -> 82 0.14189

Excited State 14: Singlet-A 5.0425 eV 245.88 nm f=0.2221 <S**2>=0.000
77 -> 81 -0.38336
78 -> 83 -0.16111
79 -> 83 -0.34524
79 -> 84 0.42600

Excited State 15: Singlet-A 5.1793 eV 239.38 nm f=0.0528 <S**2>=0.000
78 -> 81 -0.10370
78 -> 83 0.38767
79 -> 83 0.28463
79 -> 84 0.45278
79 -> 86 0.11603

Excited State 16: Singlet-A 5.2301 eV 237.06 nm f=0.0030 <S**2>=0.000
79 -> 85 0.67069
79 -> 89 -0.12556

Excited State 17: Singlet-A 5.3188 eV 233.10 nm f=0.0173 <S**2>=0.000
74 -> 81 -0.11955

75 -> 81 -0.11934
78 -> 84 -0.30437
78 -> 86 -0.17978
79 -> 83 -0.12000
79 -> 86 0.55948

Excited State 18: Singlet-A 5.3491 eV 231.78 nm f=0.1503 <S**2>=0.000
77 -> 81 -0.14680
78 -> 84 0.56685
79 -> 84 -0.17573
79 -> 86 0.30966

Excited State 19: Singlet-A 5.4172 eV 228.87 nm f=0.5118 <S**2>=0.000
75 -> 81 0.23320
77 -> 81 -0.29983
78 -> 83 0.41206
78 -> 84 -0.16987
78 -> 85 -0.11201
78 -> 86 0.18657
79 -> 81 0.10061
79 -> 83 -0.13025
79 -> 84 -0.17670

Excited State 20: Singlet-A 5.4360 eV 228.08 nm f=0.0261 <S**2>=0.000
77 -> 82 0.12707
78 -> 85 0.50342
78 -> 87 -0.17992
79 -> 87 0.39305

Excited State 21: Singlet-A 5.4538 eV 227.34 nm f=0.0161 <S**2>=0.000
76 -> 81 -0.16273
76 -> 84 -0.16201
77 -> 82 0.62248
78 -> 85 -0.10370

Excited State 22: Singlet-A 5.5488 eV 223.44 nm f=0.1506 <S**2>=0.000
74 -> 81 0.15858
78 -> 83 -0.12651
78 -> 86 0.60064
79 -> 84 0.11048
79 -> 86 0.19008

Excited State 23: Singlet-A 5.5783 eV 222.26 nm f=0.0044 <S**2>=0.000
78 -> 85 -0.40867
78 -> 89 0.14358
79 -> 87 0.52714

Excited State 24: Singlet-A 5.6128 eV 220.90 nm f=0.0164 <S**2>=0.000
70 -> 80 0.66785

Excited State 25: Singlet-A 5.7241 eV 216.60 nm f=0.0020 <S**2>=0.000
77 -> 85 0.11360
78 -> 87 0.60676
79 -> 87 0.15461
79 -> 88 0.14501
79 -> 89 0.20885

Excited State 26: Singlet-A 5.7527 eV 215.52 nm f=0.0213 <S**2>=0.000
76 -> 81 0.65295

77 -> 82 0.14896
79 -> 88 0.15624

Excited State 27: Singlet-A 5.7614 eV 215.20 nm f=0.0027 <S**2>=0.000
76 -> 81 -0.17239
78 -> 88 -0.14428
79 -> 88 0.60148
79 -> 89 -0.23225

Excited State 28: Singlet-A 5.8706 eV 211.19 nm f=0.0039 <S**2>=0.000
78 -> 87 -0.22855
78 -> 89 0.17257
79 -> 85 0.15913
79 -> 88 0.17158
79 -> 89 0.57076

Excited State 29: Singlet-A 5.9308 eV 209.05 nm f=0.1589 <S**2>=0.000
70 -> 80 0.10996
75 -> 81 -0.21507
77 -> 83 -0.33570
77 -> 84 0.35954
78 -> 83 0.11641
78 -> 88 -0.25405
78 -> 89 0.13152
79 -> 91 0.19248

Excited State 30: Singlet-A 5.9535 eV 208.25 nm f=0.0072 <S**2>=0.000
72 -> 80 0.18370
77 -> 83 -0.17830
77 -> 84 0.16704
78 -> 88 0.50507
78 -> 89 -0.20167
79 -> 88 0.17102
79 -> 90 0.22267

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8516 eV 434.79 nm f=0.5880 <S**2>=0.000
79 -> 80 0.70369
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.53692771
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1205 eV 397.32 nm f=0.1477 <S**2>=0.000
78 -> 80 0.70304

Excited State 3: Singlet-A 3.7988 eV 326.37 nm f=0.0523 <S**2>=0.000
73 -> 80 0.56504
74 -> 80 0.22778
75 -> 80 -0.21447
77 -> 80 0.24052

Excited State 4: Singlet-A 3.8836 eV 319.25 nm f=0.3166 <S**2>=0.000
73 -> 80 -0.26093
77 -> 80 0.57323
79 -> 81 0.29115

Excited State 5: Singlet-A 4.0153 eV 308.78 nm f=0.0864 <S**2>=0.000
77 -> 80 -0.30179
78 -> 83 -0.16654
79 -> 81 0.58229
79 -> 83 -0.11288

Excited State 6: Singlet-A 4.0289 eV 307.74 nm f=0.0116 <S**2>=0.000
76 -> 80 0.68383
79 -> 82 -0.12471

Excited State 7: Singlet-A 4.2572 eV 291.23 nm f=0.0504 <S**2>=0.000
78 -> 81 0.63295
79 -> 81 0.16757
79 -> 83 0.22487

Excited State 8: Singlet-A 4.4694 eV 277.41 nm f=0.0006 <S**2>=0.000
70 -> 80 0.67955
72 -> 80 0.13346

Excited State 9: Singlet-A 4.6066 eV 269.15 nm f=0.0408 <S**2>=0.000
73 -> 80 0.21725
74 -> 80 -0.17068
75 -> 80 0.49676
79 -> 82 0.32621
79 -> 83 0.13045

Excited State 10: Singlet-A 4.6298 eV 267.79 nm f=0.0072 <S**2>=0.000
73 -> 80 -0.13596
74 -> 80 0.10890
75 -> 80 -0.31217
76 -> 80 0.11494
78 -> 82 -0.14229
79 -> 82 0.56187

Excited State 11: Singlet-A 4.7590 eV 260.53 nm f=0.4376 <S**2>=0.000
77 -> 81 0.34752
78 -> 81 -0.21522
78 -> 83 0.15286
78 -> 84 0.14967
79 -> 81 0.10845
79 -> 82 -0.12178
79 -> 83 0.46997

Excited State 12: Singlet-A 4.9425 eV 250.85 nm f=0.0011 <S**2>=0.000
73 -> 80 -0.13142
74 -> 80 0.60102
75 -> 80 0.27818

Excited State 13: Singlet-A 4.9780 eV 249.06 nm f=0.0887 <S**2>=0.000
74 -> 80 0.10070
77 -> 81 0.42155
78 -> 83 0.25224
79 -> 83 -0.36569
79 -> 84 0.30240

Excited State 14: Singlet-A 5.0297 eV 246.51 nm f=0.0036 <S**2>=0.000
78 -> 82 0.66295
79 -> 82 0.18475
79 -> 84 -0.10367

Excited State 15: Singlet-A 5.1426 eV 241.09 nm f=0.0457 <S**2>=0.000
78 -> 82 0.11203
78 -> 83 -0.32583
79 -> 83 0.14906
79 -> 84 0.47537
79 -> 85 -0.27913
79 -> 86 0.10654

Excited State 16: Singlet-A 5.1675 eV 239.93 nm f=0.0295 <S**2>=0.000
78 -> 83 -0.16532
79 -> 84 0.21004
79 -> 85 0.61407
79 -> 88 0.12184

Excited State 17: Singlet-A 5.2967 eV 234.08 nm f=0.0286 <S**2>=0.000
74 -> 81 0.10254
75 -> 81 0.10760
78 -> 83 0.10330
78 -> 84 0.11543
78 -> 86 0.16629
79 -> 86 0.62725

Excited State 18: Singlet-A 5.3514 eV 231.69 nm f=0.0596 <S**2>=0.000
78 -> 83 -0.15950
78 -> 84 0.64261
79 -> 83 -0.10960
79 -> 86 -0.12530

Excited State 19: Singlet-A 5.4095 eV 229.20 nm f=0.0328 <S**2>=0.000
78 -> 85 -0.46115
78 -> 87 0.15832
79 -> 87 0.47547

Excited State 20: Singlet-A 5.4641 eV 226.90 nm f=0.4013 <S**2>=0.000
72 -> 80 0.23437
75 -> 81 0.24055
77 -> 81 -0.32320
78 -> 83 0.32661
78 -> 86 0.22730
79 -> 84 0.21155

Excited State 21: Singlet-A 5.5040 eV 225.26 nm f=0.0068 <S**2>=0.000
70 -> 80 -0.12317
72 -> 80 0.59799
75 -> 81 -0.11583
78 -> 86 -0.22953
79 -> 86 0.10455

Excited State 22: Singlet-A 5.5513 eV 223.34 nm f=0.0064 <S**2>=0.000
78 -> 85 0.44467
78 -> 89 0.10043
79 -> 87 0.40840
79 -> 88 0.28037

Excited State 23: Singlet-A 5.5596 eV 223.01 nm f=0.0750 <S**2>=0.000
74 -> 81 0.13456
76 -> 81 -0.34240
77 -> 82 0.30111

78 -> 86 0.40476
79 -> 86 -0.10058

Excited State 24: Singlet-A 5.5763 eV 222.34 nm f=0.2343 <S**2>=0.000
72 -> 80 0.12284
74 -> 81 0.13205
76 -> 81 0.39687
77 -> 81 0.13902
77 -> 82 -0.25030
78 -> 83 -0.12916
78 -> 84 -0.10420
78 -> 86 0.34748
79 -> 84 -0.11942

Excited State 25: Singlet-A 5.5984 eV 221.46 nm f=0.0022 <S**2>=0.000
78 -> 85 -0.16044
78 -> 87 0.16203
79 -> 85 -0.11306
79 -> 87 -0.24131
79 -> 88 0.58790

Excited State 26: Singlet-A 5.7205 eV 216.74 nm f=0.0048 <S**2>=0.000
71 -> 80 -0.16841
76 -> 81 0.43696
77 -> 82 0.48192

Excited State 27: Singlet-A 5.7297 eV 216.39 nm f=0.0021 <S**2>=0.000
78 -> 87 0.54887
79 -> 88 -0.12074
79 -> 89 0.35439

Excited State 28: Singlet-A 5.8106 eV 213.37 nm f=0.0009 <S**2>=0.000
78 -> 87 -0.24113
78 -> 88 -0.37756
79 -> 89 0.48520
79 -> 90 0.15889

Excited State 29: Singlet-A 5.8939 eV 210.36 nm f=0.0115 <S**2>=0.000
78 -> 87 -0.19515
78 -> 88 0.40662
78 -> 89 -0.25025
79 -> 89 0.31307
79 -> 90 -0.32133

Excited State 30: Singlet-A 5.9322 eV 209.00 nm f=0.0673 <S**2>=0.000
71 -> 80 0.63573
75 -> 81 -0.11049
77 -> 82 0.11941

Single-point TDDFT X3LYP/6-311++G(2df,2p)/PCM(DMSO) over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometry

1

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8154 eV 440.37 nm f=0.2421 <S**2>=0.000

79 -> 80 0.70450
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.09582764
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2138 eV 385.79 nm f=0.4555 <S**2>=0.000
78 -> 80 0.70066

Excited State 3: Singlet-A 3.8566 eV 321.49 nm f=0.0000 <S**2>=0.000
73 -> 80 -0.30093
74 -> 80 0.62481

Excited State 4: Singlet-A 4.0211 eV 308.34 nm f=0.2943 <S**2>=0.000
77 -> 80 -0.33288
79 -> 81 0.60135

Excited State 5: Singlet-A 4.1152 eV 301.28 nm f=0.1407 <S**2>=0.000
76 -> 80 0.13363
77 -> 80 0.59500
79 -> 81 0.31184
79 -> 83 0.11380

Excited State 6: Singlet-A 4.1771 eV 296.82 nm f=0.0105 <S**2>=0.000
76 -> 80 0.64963
77 -> 80 -0.12187
77 -> 82 -0.10093
78 -> 82 -0.12134
79 -> 82 -0.14003

Excited State 7: Singlet-A 4.2282 eV 293.23 nm f=0.0485 <S**2>=0.000
78 -> 81 0.58832
79 -> 81 -0.11244
79 -> 83 0.31118
79 -> 85 -0.12599

Excited State 8: Singlet-A 4.4854 eV 276.42 nm f=0.0004 <S**2>=0.000
70 -> 80 0.67209
73 -> 80 0.15636

Excited State 9: Singlet-A 4.5505 eV 272.46 nm f=0.0536 <S**2>=0.000
76 -> 80 0.17205
78 -> 81 -0.10556
78 -> 82 0.13976
79 -> 82 0.65596

Excited State 10: Singlet-A 4.8166 eV 257.41 nm f=0.0292 <S**2>=0.000
75 -> 80 0.66985
79 -> 83 -0.13431

Excited State 11: Singlet-A 4.8731 eV 254.43 nm f=0.7075 <S**2>=0.000
75 -> 80 0.16829
77 -> 81 -0.22198
78 -> 81 -0.30237
78 -> 82 0.11861
78 -> 85 0.12606
79 -> 83 0.52090

Excited State 12: Singlet-A 4.9617 eV 249.88 nm f=0.1440 <S**2>=0.000
78 -> 82 0.65063

79 -> 82 -0.16311
79 -> 83 -0.10163

Excited State 13: Singlet-A 5.1040 eV 242.92 nm f=0.0002 <S**2>=0.000
70 -> 80 -0.16755
73 -> 80 0.60641
74 -> 80 0.29375

Excited State 14: Singlet-A 5.1236 eV 241.99 nm f=0.0000 <S**2>=0.000
79 -> 84 0.63488
79 -> 86 -0.25010
79 -> 89 0.12112

Excited State 15: Singlet-A 5.1695 eV 239.84 nm f=0.0061 <S**2>=0.000
75 -> 81 -0.13534
77 -> 81 0.28454
79 -> 83 0.14367
79 -> 85 0.52317
79 -> 87 -0.27997

Excited State 16: Singlet-A 5.3043 eV 233.74 nm f=0.0400 <S**2>=0.000
77 -> 81 0.36250
78 -> 83 0.36396
79 -> 83 0.15022
79 -> 87 0.42535

Excited State 17: Singlet-A 5.3428 eV 232.06 nm f=0.0006 <S**2>=0.000
78 -> 84 0.23352
79 -> 84 0.20168
79 -> 86 0.60137
79 -> 88 0.11648
79 -> 89 0.11674

Excited State 18: Singlet-A 5.3918 eV 229.95 nm f=0.0225 <S**2>=0.000
77 -> 81 0.10189
78 -> 83 0.43086
79 -> 85 -0.30419
79 -> 87 -0.42466

Excited State 19: Singlet-A 5.5470 eV 223.52 nm f=0.0001 <S**2>=0.000
78 -> 84 -0.38028
79 -> 88 0.53254
79 -> 89 -0.12146
79 -> 90 0.17142

Excited State 20: Singlet-A 5.5483 eV 223.46 nm f=0.0250 <S**2>=0.000
72 -> 80 0.66963
77 -> 81 0.11955

Excited State 21: Singlet-A 5.5694 eV 222.62 nm f=0.0013 <S**2>=0.000
78 -> 84 0.49022
78 -> 89 0.10050
79 -> 86 -0.18551
79 -> 88 0.31013
79 -> 89 -0.29349

Excited State 22: Singlet-A 5.6158 eV 220.78 nm f=0.0168 <S**2>=0.000
75 -> 83 0.13045
78 -> 85 0.58901

78 -> 87 -0.27817

Excited State 23: Singlet-A 5.6848 eV 218.10 nm f=0.3904 <S**2>=0.000
72 -> 80 0.10506
76 -> 81 0.12707
77 -> 81 -0.29182
77 -> 82 0.42043
78 -> 83 0.28448
79 -> 83 -0.11037
79 -> 85 0.19242

Excited State 24: Singlet-A 5.6995 eV 217.54 nm f=0.0010 <S**2>=0.000
78 -> 86 -0.33195
79 -> 84 -0.14943
79 -> 86 -0.14439
79 -> 88 0.20168
79 -> 89 0.51204
79 -> 91 0.10375

Excited State 25: Singlet-A 5.7644 eV 215.09 nm f=0.3176 <S**2>=0.000
76 -> 81 0.35290
77 -> 81 0.28395
77 -> 82 0.36116
78 -> 82 -0.11137
78 -> 83 -0.21633
79 -> 83 0.10835
79 -> 85 -0.18775

Excited State 26: Singlet-A 5.8018 eV 213.70 nm f=0.0033 <S**2>=0.000
78 -> 86 0.44012
78 -> 88 0.23487
79 -> 84 -0.11056
79 -> 88 0.18712
79 -> 89 0.21323
79 -> 90 -0.36736

Excited State 27: Singlet-A 5.8070 eV 213.51 nm f=0.1593 <S**2>=0.000
75 -> 81 -0.21671
78 -> 85 0.29377
78 -> 87 0.53826
79 -> 85 -0.10908

Excited State 28: Singlet-A 5.8476 eV 212.02 nm f=0.0005 <S**2>=0.000
78 -> 84 0.11269
78 -> 86 0.39111
78 -> 88 -0.13299
79 -> 89 0.16973
79 -> 90 0.49125

Excited State 29: Singlet-A 5.9065 eV 209.91 nm f=0.0152 <S**2>=0.000
71 -> 80 0.20919
75 -> 81 0.40817
76 -> 81 0.37459
77 -> 82 -0.16617
78 -> 87 0.23325
79 -> 93 0.13570

Excited State 30: Singlet-A 5.9548 eV 208.21 nm f=0.0358 <S**2>=0.000
71 -> 80 -0.40968

75 -> 81 0.42051
76 -> 81 -0.29640
77 -> 82 0.12612
78 -> 87 0.10432

1-

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5108 eV 493.79 nm f=0.9802 <S**2>=0.000
79 -> 80 0.70493
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.63964410
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0592 eV 405.28 nm f=0.1959 <S**2>=0.000
78 -> 80 0.69899

Excited State 3: Singlet-A 3.6308 eV 341.48 nm f=0.2544 <S**2>=0.000
77 -> 80 -0.21106
79 -> 81 0.65679

Excited State 4: Singlet-A 3.7785 eV 328.13 nm f=0.0000 <S**2>=0.000
72 -> 80 0.60089
73 -> 80 -0.16091
76 -> 80 -0.30790

Excited State 5: Singlet-A 3.9054 eV 317.47 nm f=0.0698 <S**2>=0.000
77 -> 80 0.64277
78 -> 83 -0.10348
79 -> 81 0.17629
79 -> 83 0.15871

Excited State 6: Singlet-A 4.0337 eV 307.37 nm f=0.0051 <S**2>=0.000
75 -> 80 0.53207
79 -> 82 -0.44084

Excited State 7: Singlet-A 4.0659 eV 304.93 nm f=0.0002 <S**2>=0.000
72 -> 80 0.29793
76 -> 80 0.62848

Excited State 8: Singlet-A 4.1497 eV 298.78 nm f=0.0042 <S**2>=0.000
75 -> 80 0.32183
77 -> 80 -0.11218
78 -> 81 0.45149
79 -> 82 0.35202
79 -> 83 0.19231

Excited State 9: Singlet-A 4.2064 eV 294.75 nm f=0.0703 <S**2>=0.000
75 -> 80 0.30937
78 -> 81 -0.39714
79 -> 82 0.40112
79 -> 83 -0.25988

Excited State 10: Singlet-A 4.4648 eV 277.69 nm f=0.0007 <S**2>=0.000
79 -> 84 0.66777
79 -> 85 0.15582
79 -> 88 -0.13065

Excited State 11: Singlet-A 4.5225 eV 274.15 nm f=0.4071 <S**2>=0.000
77 -> 80 -0.12760
77 -> 81 -0.11482
78 -> 81 -0.31863
79 -> 83 0.56223
79 -> 86 0.14370

Excited State 12: Singlet-A 4.5252 eV 273.98 nm f=0.0002 <S**2>=0.000
69 -> 80 0.60337
73 -> 80 -0.33015

Excited State 13: Singlet-A 4.6850 eV 264.64 nm f=0.0006 <S**2>=0.000
69 -> 80 0.33721
72 -> 80 0.14410
73 -> 80 0.59180

Excited State 14: Singlet-A 4.7102 eV 263.22 nm f=0.0048 <S**2>=0.000
78 -> 84 0.13362
79 -> 84 -0.13584
79 -> 85 0.66372

Excited State 15: Singlet-A 4.7402 eV 261.56 nm f=0.0020 <S**2>=0.000
74 -> 80 0.39307
78 -> 81 0.10451
79 -> 86 0.54536

Excited State 16: Singlet-A 4.8250 eV 256.96 nm f=0.0298 <S**2>=0.000
74 -> 80 0.13811
77 -> 81 0.41495
78 -> 82 0.24700
78 -> 83 0.36971
79 -> 83 0.19076
79 -> 86 -0.14917
79 -> 89 0.13199

Excited State 17: Singlet-A 4.8630 eV 254.96 nm f=0.0312 <S**2>=0.000
74 -> 80 0.55128
77 -> 81 -0.20327
79 -> 86 -0.32882
79 -> 89 0.12084

Excited State 18: Singlet-A 4.9197 eV 252.01 nm f=0.0010 <S**2>=0.000
79 -> 87 0.67932
79 -> 90 0.12112

Excited State 19: Singlet-A 4.9820 eV 248.87 nm f=0.0002 <S**2>=0.000
78 -> 85 0.12144
79 -> 84 0.14145
79 -> 88 0.66536

Excited State 20: Singlet-A 5.0363 eV 246.18 nm f=0.1163 <S**2>=0.000
77 -> 81 0.13450
78 -> 82 -0.35154
79 -> 89 0.56184

Excited State 21: Singlet-A 5.0561 eV 245.22 nm f=0.0065 <S**2>=0.000
78 -> 82 0.52958
78 -> 83 -0.26624

78 -> 86 0.15072
79 -> 86 0.10927
79 -> 89 0.28699

Excited State 22: Singlet-A 5.0986 eV 243.17 nm f=0.0008 <S**2>=0.000
78 -> 84 0.61592
78 -> 85 -0.25021
78 -> 88 -0.11028
79 -> 85 -0.12538

Excited State 23: Singlet-A 5.1847 eV 239.13 nm f=0.0000 <S**2>=0.000
78 -> 87 0.13553
79 -> 87 -0.11615
79 -> 90 0.67558

Excited State 24: Singlet-A 5.2712 eV 235.21 nm f=0.0051 <S**2>=0.000
71 -> 80 -0.20518
74 -> 81 0.10485
78 -> 83 0.20859
78 -> 86 0.58048
78 -> 89 -0.17239
79 -> 89 -0.11284

Excited State 25: Singlet-A 5.3304 eV 232.60 nm f=0.0526 <S**2>=0.000
71 -> 80 0.62637
77 -> 81 0.16183
78 -> 86 0.23774

Excited State 26: Singlet-A 5.3689 eV 230.93 nm f=0.0003 <S**2>=0.000
78 -> 84 0.18258
78 -> 85 0.57895
78 -> 88 -0.28341
79 -> 91 0.14538

Excited State 27: Singlet-A 5.4741 eV 226.49 nm f=0.0003 <S**2>=0.000
76 -> 81 0.66885
79 -> 91 0.11974

Excited State 28: Singlet-A 5.4887 eV 225.89 nm f=0.0001 <S**2>=0.000
76 -> 81 -0.12475
78 -> 87 0.44754
79 -> 91 0.47169
79 -> 93 -0.11176

Excited State 29: Singlet-A 5.5004 eV 225.41 nm f=0.0000 <S**2>=0.000
78 -> 84 0.15025
78 -> 85 0.15395
78 -> 87 0.47393
78 -> 90 -0.10729
79 -> 91 -0.41660

Excited State 30: Singlet-A 5.5554 eV 223.18 nm f=0.8475 <S**2>=0.000
71 -> 80 0.16131
77 -> 81 -0.40772
77 -> 82 0.14809
78 -> 83 0.41485
79 -> 89 0.16957
79 -> 94 -0.11687

1’

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7699 eV 447.61 nm f=0.3910 <S**2>=0.000
79 -> 80 0.70585
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.09504450
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2281 eV 384.07 nm f=0.3586 <S**2>=0.000
78 -> 80 0.70110

Excited State 3: Singlet-A 3.8541 eV 321.70 nm f=0.0000 <S**2>=0.000
74 -> 80 0.69271

Excited State 4: Singlet-A 3.9592 eV 313.16 nm f=0.3192 <S**2>=0.000
77 -> 80 -0.19847
79 -> 81 0.65570

Excited State 5: Singlet-A 4.0951 eV 302.76 nm f=0.1098 <S**2>=0.000
77 -> 80 0.65723
79 -> 81 0.17785
79 -> 83 0.11791

Excited State 6: Singlet-A 4.1868 eV 296.13 nm f=0.0075 <S**2>=0.000
76 -> 80 0.63870
77 -> 82 0.10090
78 -> 82 0.12560
79 -> 82 0.21778

Excited State 7: Singlet-A 4.2483 eV 291.85 nm f=0.0262 <S**2>=0.000
78 -> 81 0.57877
79 -> 81 -0.10843
79 -> 83 0.32876
79 -> 85 -0.13821

Excited State 8: Singlet-A 4.4778 eV 276.89 nm f=0.0169 <S**2>=0.000
76 -> 80 -0.24203
79 -> 82 0.64914

Excited State 9: Singlet-A 4.4912 eV 276.06 nm f=0.0004 <S**2>=0.000
70 -> 80 0.69267

Excited State 10: Singlet-A 4.8060 eV 257.98 nm f=0.6917 <S**2>=0.000
75 -> 80 -0.15963
77 -> 81 -0.20296
78 -> 81 -0.34239
78 -> 82 0.11533
78 -> 85 0.10682
79 -> 83 0.51341

Excited State 11: Singlet-A 4.8332 eV 256.52 nm f=0.0548 <S**2>=0.000
75 -> 80 0.67371
79 -> 83 0.13042

Excited State 12: Singlet-A 4.9656 eV 249.69 nm f=0.0618 <S**2>=0.000
78 -> 82 0.64792
79 -> 82 -0.12538

79 -> 83 -0.14424
79 -> 85 -0.13241

Excited State 13: Singlet-A 5.0348 eV 246.25 nm f=0.0003 <S**2>=0.000
79 -> 84 0.66022
79 -> 86 -0.15816
79 -> 88 -0.10608
79 -> 89 0.11122

Excited State 14: Singlet-A 5.1237 eV 241.98 nm f=0.0081 <S**2>=0.000
75 -> 81 -0.11711
77 -> 81 0.34005
78 -> 82 0.14205
79 -> 83 0.13955
79 -> 85 0.49202
79 -> 87 -0.23316

Excited State 15: Singlet-A 5.2541 eV 235.98 nm f=0.0148 <S**2>=0.000
77 -> 81 0.33625
78 -> 83 0.31690
79 -> 83 0.13485
79 -> 87 0.48486

Excited State 16: Singlet-A 5.2611 eV 235.66 nm f=0.0002 <S**2>=0.000
73 -> 80 0.69459
73 -> 81 -0.10299

Excited State 17: Singlet-A 5.2741 eV 235.08 nm f=0.0011 <S**2>=0.000
78 -> 84 0.18489
79 -> 84 0.12024
79 -> 86 0.64693

Excited State 18: Singlet-A 5.3620 eV 231.23 nm f=0.0393 <S**2>=0.000
77 -> 81 0.13582
78 -> 83 0.44237
79 -> 85 -0.31530
79 -> 87 -0.39496

Excited State 19: Singlet-A 5.5023 eV 225.33 nm f=0.0000 <S**2>=0.000
79 -> 84 0.10310
79 -> 88 0.64851
79 -> 89 0.12533
79 -> 90 -0.19239

Excited State 20: Singlet-A 5.5517 eV 223.33 nm f=0.0271 <S**2>=0.000
72 -> 80 0.66801
77 -> 81 0.12419
78 -> 83 -0.12478

Excited State 21: Singlet-A 5.5691 eV 222.63 nm f=0.0004 <S**2>=0.000
78 -> 84 0.61588
78 -> 89 0.12236
79 -> 86 -0.14996
79 -> 89 -0.22017

Excited State 22: Singlet-A 5.6251 eV 220.41 nm f=0.0406 <S**2>=0.000
75 -> 83 0.13122
77 -> 83 -0.11206
78 -> 83 0.10397

78 -> 85 0.57284
78 -> 87 -0.26623
79 -> 85 0.13102

Excited State 23: Singlet-A 5.6652 eV 218.85 nm f=0.0011 <S**2>=0.000
78 -> 84 0.17116
78 -> 86 -0.26049
79 -> 84 -0.13392
79 -> 86 -0.11769
79 -> 89 0.57576

Excited State 24: Singlet-A 5.6742 eV 218.50 nm f=0.3526 <S**2>=0.000
72 -> 80 0.13558
76 -> 81 -0.14929
77 -> 81 -0.27013
77 -> 82 0.44864
78 -> 83 0.25613
79 -> 85 0.19579

Excited State 25: Singlet-A 5.7569 eV 215.37 nm f=0.0013 <S**2>=0.000
78 -> 86 -0.13743
78 -> 88 0.19346
79 -> 88 0.19095
79 -> 89 -0.11048
79 -> 90 0.60840

Excited State 26: Singlet-A 5.7671 eV 214.99 nm f=0.3917 <S**2>=0.000
76 -> 81 -0.30707
77 -> 81 0.28484
77 -> 82 0.34438
78 -> 83 -0.26144
78 -> 87 -0.15752
79 -> 85 -0.18866

Excited State 27: Singlet-A 5.8267 eV 212.79 nm f=0.1713 <S**2>=0.000
75 -> 81 -0.30227
78 -> 85 0.30617
78 -> 87 0.49870

Excited State 28: Singlet-A 5.8418 eV 212.23 nm f=0.0045 <S**2>=0.000
78 -> 84 0.12904
78 -> 86 0.60969
79 -> 89 0.19676
79 -> 90 0.17076

Excited State 29: Singlet-A 5.9351 eV 208.90 nm f=0.0566 <S**2>=0.000
71 -> 80 0.47523
76 -> 81 -0.46137
77 -> 82 -0.16520

Excited State 30: Singlet-A 5.9586 eV 208.08 nm f=0.0119 <S**2>=0.000
75 -> 81 0.56303
78 -> 87 0.31060
79 -> 93 0.16712

1'-

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4862 eV 498.69 nm f=1.0291 <S**2>=0.000
79 -> 80 0.70485
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.63761536
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0857 eV 401.80 nm f=0.1283 <S**2>=0.000
78 -> 80 0.69410
79 -> 81 -0.11801

Excited State 3: Singlet-A 3.5563 eV 348.63 nm f=0.2612 <S**2>=0.000
77 -> 80 0.33516
78 -> 80 0.10082
79 -> 81 0.59895

Excited State 4: Singlet-A 3.7385 eV 331.64 nm f=0.0305 <S**2>=0.000
72 -> 80 0.30513
74 -> 80 0.10806
75 -> 80 -0.14853
76 -> 80 0.16486
77 -> 80 0.47381
79 -> 81 -0.29387
79 -> 83 0.10375

Excited State 5: Singlet-A 3.8164 eV 324.87 nm f=0.0174 <S**2>=0.000
72 -> 80 0.56746
74 -> 80 0.10147
77 -> 80 -0.33761
79 -> 81 0.12047

Excited State 6: Singlet-A 4.0197 eV 308.44 nm f=0.0006 <S**2>=0.000
75 -> 80 0.25993
76 -> 80 0.26585
79 -> 82 0.58763

Excited State 7: Singlet-A 4.1433 eV 299.24 nm f=0.0238 <S**2>=0.000
76 -> 80 0.38372
78 -> 81 -0.35077
79 -> 82 -0.21139
79 -> 83 -0.37648

Excited State 8: Singlet-A 4.1743 eV 297.02 nm f=0.0180 <S**2>=0.000
75 -> 80 0.37660
76 -> 80 0.30892
78 -> 81 0.31489
79 -> 82 -0.30168
79 -> 83 0.23050

Excited State 9: Singlet-A 4.2594 eV 291.09 nm f=0.0073 <S**2>=0.000
72 -> 80 0.19484
75 -> 80 0.47203
76 -> 80 -0.33325
77 -> 80 0.14239
78 -> 81 -0.27533

Excited State 10: Singlet-A 4.3845 eV 282.78 nm f=0.0351 <S**2>=0.000
78 -> 81 -0.13455
79 -> 83 0.22657
79 -> 84 0.61991

79 -> 85 0.10571
79 -> 88 -0.10721

Excited State 11: Singlet-A 4.4772 eV 276.93 nm f=0.3652 <S**2>=0.000
76 -> 80 0.11245
77 -> 80 -0.12815
77 -> 81 0.10262
78 -> 81 -0.37077
79 -> 83 0.43732
79 -> 84 -0.26660
79 -> 86 0.16592

Excited State 12: Singlet-A 4.5549 eV 272.20 nm f=0.0007 <S**2>=0.000
69 -> 80 0.69038

Excited State 13: Singlet-A 4.6540 eV 266.40 nm f=0.0063 <S**2>=0.000
78 -> 84 -0.11426
79 -> 85 0.67165

Excited State 14: Singlet-A 4.7021 eV 263.68 nm f=0.0229 <S**2>=0.000
74 -> 80 -0.21468
77 -> 81 -0.14448
78 -> 81 0.14612
79 -> 86 0.60276
79 -> 89 -0.11529

Excited State 15: Singlet-A 4.7795 eV 259.41 nm f=0.0028 <S**2>=0.000
73 -> 80 0.14575
77 -> 81 0.47801
78 -> 83 0.32010
79 -> 83 -0.13032
79 -> 87 0.21216
79 -> 89 -0.20734

Excited State 16: Singlet-A 4.8016 eV 258.21 nm f=0.0006 <S**2>=0.000
73 -> 80 0.67582
77 -> 81 -0.11818

Excited State 17: Singlet-A 4.8547 eV 255.39 nm f=0.0032 <S**2>=0.000
74 -> 80 0.11582
77 -> 81 -0.12143
78 -> 83 -0.12621
79 -> 87 0.60085
79 -> 88 0.20130

Excited State 18: Singlet-A 4.8942 eV 253.33 nm f=0.0026 <S**2>=0.000
74 -> 80 0.57602
75 -> 80 0.10472
76 -> 80 -0.10430
79 -> 86 0.14943
79 -> 88 -0.21955
79 -> 89 -0.17811

Excited State 19: Singlet-A 4.9399 eV 250.98 nm f=0.0029 <S**2>=0.000
74 -> 80 0.14294
78 -> 85 -0.10378
79 -> 84 0.10031
79 -> 87 -0.23294
79 -> 88 0.58883

79 -> 89 -0.16234

Excited State 20: Singlet-A 5.0007 eV 247.94 nm f=0.0593 <S**2>=0.000
74 -> 80 0.17555
78 -> 82 0.30169
78 -> 83 0.19734
79 -> 86 0.13398
79 -> 89 0.52680

Excited State 21: Singlet-A 5.0336 eV 246.31 nm f=0.0265 <S**2>=0.000
78 -> 82 0.60408
78 -> 83 -0.10437
78 -> 84 0.11157
79 -> 86 -0.12470
79 -> 89 -0.22728

Excited State 22: Singlet-A 5.1252 eV 241.91 nm f=0.0040 <S**2>=0.000
78 -> 87 0.10348
79 -> 90 0.66777

Excited State 23: Singlet-A 5.1344 eV 241.48 nm f=0.0017 <S**2>=0.000
78 -> 82 -0.11223
78 -> 83 0.10869
78 -> 84 0.61531
78 -> 85 -0.20870
78 -> 88 -0.10602
79 -> 85 0.11256

Excited State 24: Singlet-A 5.2861 eV 234.55 nm f=0.3873 <S**2>=0.000
71 -> 80 0.29021
75 -> 81 0.17005
76 -> 81 -0.18624
77 -> 81 -0.30326
78 -> 83 0.38640
78 -> 85 0.10372
78 -> 86 0.20562

Excited State 25: Singlet-A 5.3175 eV 233.16 nm f=0.0775 <S**2>=0.000
71 -> 80 -0.12685
75 -> 81 -0.12384
76 -> 81 0.17564
77 -> 81 0.15176
78 -> 85 0.15111
78 -> 86 0.56411
78 -> 89 -0.10500

Excited State 26: Singlet-A 5.3782 eV 230.53 nm f=0.0075 <S**2>=0.000
71 -> 80 -0.22985
78 -> 84 0.10899
78 -> 85 0.49701
78 -> 86 -0.15338
78 -> 88 -0.18990
78 -> 89 0.11547
79 -> 91 -0.27297

Excited State 27: Singlet-A 5.4058 eV 229.35 nm f=0.0652 <S**2>=0.000
71 -> 80 0.53166
75 -> 81 -0.13532
76 -> 81 0.17645

78 -> 83 -0.11334
78 -> 85 0.22591

Excited State 28: Singlet-A 5.4415 eV 227.85 nm f=0.0040 <S**2>=0.000
71 -> 80 -0.10755
78 -> 84 0.12604
78 -> 85 0.23229
79 -> 91 0.58337

Excited State 29: Singlet-A 5.5170 eV 224.73 nm f=0.0312 <S**2>=0.000
76 -> 82 0.10558
77 -> 82 0.38540
78 -> 87 -0.22100
79 -> 91 0.14698
79 -> 92 0.37160
79 -> 93 0.12995
79 -> 94 -0.23330

Excited State 30: Singlet-A 5.5329 eV 224.08 nm f=0.0011 <S**2>=0.000
75 -> 81 0.20279
76 -> 82 0.10337
77 -> 82 0.46701
78 -> 87 0.12131
79 -> 91 -0.10175
79 -> 92 -0.32642
79 -> 93 -0.10222
79 -> 94 0.16339

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9233 eV 424.12 nm f=0.3676 <S**2>=0.000
78 -> 80 0.12231
79 -> 80 0.69265
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.08524502
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1807 eV 389.80 nm f=0.1642 <S**2>=0.000
78 -> 80 0.69287
79 -> 80 -0.12644

Excited State 3: Singlet-A 3.8290 eV 323.81 nm f=0.1743 <S**2>=0.000
73 -> 80 0.50103
74 -> 80 0.14714
75 -> 80 -0.13943
77 -> 80 0.42376
79 -> 81 0.10746

Excited State 4: Singlet-A 3.8787 eV 319.65 nm f=0.2163 <S**2>=0.000
73 -> 80 -0.43506
77 -> 80 0.51921
79 -> 81 0.13383

Excited State 5: Singlet-A 4.0997 eV 302.42 nm f=0.1469 <S**2>=0.000
76 -> 80 0.20362
77 -> 80 -0.15562
78 -> 81 0.18192

78 -> 83 -0.17849
79 -> 81 0.57543
79 -> 83 0.13928

Excited State 6: Singlet-A 4.1263 eV 300.47 nm f=0.0343 <S**2>=0.000
76 -> 80 0.64510
77 -> 82 -0.10375
79 -> 81 -0.16592
79 -> 82 -0.12326

Excited State 7: Singlet-A 4.2802 eV 289.67 nm f=0.0572 <S**2>=0.000
78 -> 81 0.60735
79 -> 81 -0.25648
79 -> 83 0.22111

Excited State 8: Singlet-A 4.4944 eV 275.86 nm f=0.0005 <S**2>=0.000
70 -> 80 0.10186
71 -> 80 0.68684

Excited State 9: Singlet-A 4.6237 eV 268.15 nm f=0.0123 <S**2>=0.000
76 -> 80 0.15564
78 -> 82 0.23321
79 -> 82 0.63491

Excited State 10: Singlet-A 4.7515 eV 260.94 nm f=0.0699 <S**2>=0.000
73 -> 80 0.16355
74 -> 80 -0.24424
75 -> 80 0.57559
79 -> 83 -0.15466

Excited State 11: Singlet-A 4.8529 eV 255.48 nm f=0.4155 <S**2>=0.000
74 -> 80 0.10391
75 -> 80 -0.18457
77 -> 81 0.40907
78 -> 81 0.21247
78 -> 83 0.15649
78 -> 84 0.14039
79 -> 81 0.10953
79 -> 83 -0.38877

Excited State 12: Singlet-A 4.9960 eV 248.17 nm f=0.0025 <S**2>=0.000
78 -> 82 0.64417
79 -> 82 -0.25453

Excited State 13: Singlet-A 5.0320 eV 246.39 nm f=0.0012 <S**2>=0.000
74 -> 80 0.60989
75 -> 80 0.29796

Excited State 14: Singlet-A 5.1051 eV 242.86 nm f=0.1932 <S**2>=0.000
77 -> 81 -0.39534
78 -> 83 -0.18034
79 -> 83 -0.32968
79 -> 84 0.40988

Excited State 15: Singlet-A 5.1704 eV 239.79 nm f=0.0024 <S**2>=0.000
79 -> 84 0.15534
79 -> 85 0.65245
79 -> 89 -0.13011

Excited State 16: Singlet-A 5.2332 eV 236.92 nm f=0.0534 <S**2>=0.000
78 -> 81 -0.10610
78 -> 83 0.37194
79 -> 83 0.27568
79 -> 84 0.42831
79 -> 85 -0.15848
79 -> 86 0.15155

Excited State 17: Singlet-A 5.3424 eV 232.07 nm f=0.0123 <S**2>=0.000
74 -> 81 -0.10855
78 -> 84 -0.19782
78 -> 86 -0.17779
79 -> 83 -0.12461
79 -> 86 0.59700

Excited State 18: Singlet-A 5.3875 eV 230.13 nm f=0.0054 <S**2>=0.000
78 -> 84 0.16972
78 -> 85 0.50446
78 -> 87 -0.19089
79 -> 87 0.38659

Excited State 19: Singlet-A 5.4131 eV 229.04 nm f=0.2555 <S**2>=0.000
77 -> 81 -0.21144
78 -> 84 0.53144
78 -> 85 -0.15543
78 -> 86 0.11776
79 -> 84 -0.20738
79 -> 86 0.17790

Excited State 20: Singlet-A 5.4587 eV 227.13 nm f=0.4176 <S**2>=0.000
75 -> 81 0.20000
77 -> 81 -0.27609
78 -> 83 0.41188
78 -> 84 -0.29102
78 -> 86 0.19216
79 -> 83 -0.14521
79 -> 84 -0.12062

Excited State 21: Singlet-A 5.5032 eV 225.29 nm f=0.0161 <S**2>=0.000
75 -> 82 -0.10266
76 -> 81 -0.14785
76 -> 84 -0.16273
77 -> 82 0.63150

Excited State 22: Singlet-A 5.5422 eV 223.71 nm f=0.0018 <S**2>=0.000
78 -> 85 -0.38745
78 -> 89 0.15138
79 -> 87 0.53054
79 -> 89 -0.10837

Excited State 23: Singlet-A 5.5808 eV 222.16 nm f=0.2054 <S**2>=0.000
74 -> 81 0.14105
77 -> 81 0.10682
78 -> 83 -0.14326
78 -> 86 0.58471
79 -> 84 0.13025
79 -> 86 0.19262

Excited State 24: Singlet-A 5.6818 eV 218.21 nm f=0.0114 <S**2>=0.000

70 -> 80 0.65708
77 -> 84 -0.11126

Excited State 25: Singlet-A 5.6913 eV 217.85 nm f=0.0021 <S**2>=0.000
77 -> 85 0.12497
78 -> 87 0.59231
79 -> 87 0.16470
79 -> 88 0.10864
79 -> 89 0.23207

Excited State 26: Singlet-A 5.7250 eV 216.56 nm f=0.0016 <S**2>=0.000
78 -> 88 -0.15499
79 -> 88 0.63014
79 -> 89 -0.21656

Excited State 27: Singlet-A 5.8361 eV 212.44 nm f=0.0187 <S**2>=0.000
72 -> 80 -0.12467
76 -> 81 0.67327
77 -> 82 0.13621

Excited State 28: Singlet-A 5.8451 eV 212.12 nm f=0.0011 <S**2>=0.000
78 -> 87 -0.23656
78 -> 89 0.20330
79 -> 85 0.15988
79 -> 88 0.14829
79 -> 89 0.56299

Excited State 29: Singlet-A 5.9150 eV 209.61 nm f=0.0166 <S**2>=0.000
78 -> 88 0.57921
78 -> 89 -0.21038
79 -> 88 0.17621
79 -> 90 0.16994
79 -> 91 -0.14478

Excited State 30: Singlet-A 5.9748 eV 207.51 nm f=0.1276 <S**2>=0.000
70 -> 80 0.10106
75 -> 81 -0.32167
77 -> 83 -0.20275
77 -> 84 0.24239
78 -> 83 0.10253
79 -> 90 0.36239
79 -> 91 0.22601
79 -> 93 0.10563

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9057 eV 426.69 nm f=0.6379 <S**2>=0.000
79 -> 80 0.70043
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.08749825
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1940 eV 388.18 nm f=0.1261 <S**2>=0.000
78 -> 80 0.69978

Excited State 3: Singlet-A 3.8262 eV 324.04 nm f=0.0291 <S**2>=0.000
73 -> 80 0.60404

74 -> 80 0.20749
75 -> 80 -0.18758
77 -> 80 0.17986

Excited State 4: Singlet-A 3.9376 eV 314.88 nm f=0.3266 <S**2>=0.000
73 -> 80 -0.20528
77 -> 80 0.58564
79 -> 81 0.31143

Excited State 5: Singlet-A 4.0477 eV 306.31 nm f=0.0792 <S**2>=0.000
77 -> 80 -0.31686
78 -> 83 -0.17061
79 -> 81 0.57323
79 -> 83 -0.11450

Excited State 6: Singlet-A 4.0659 eV 304.94 nm f=0.0118 <S**2>=0.000
76 -> 80 0.68216
79 -> 82 -0.12845

Excited State 7: Singlet-A 4.2880 eV 289.14 nm f=0.0509 <S**2>=0.000
78 -> 81 0.63218
79 -> 81 0.16385
79 -> 83 0.22498

Excited State 8: Singlet-A 4.4920 eV 276.01 nm f=0.0006 <S**2>=0.000
70 -> 80 0.68876

Excited State 9: Singlet-A 4.6646 eV 265.80 nm f=0.0466 <S**2>=0.000
75 -> 80 0.21981
76 -> 80 0.12833
78 -> 82 -0.15683
79 -> 82 0.57194
79 -> 83 0.14698

Excited State 10: Singlet-A 4.6995 eV 263.83 nm f=0.0352 <S**2>=0.000
72 -> 80 -0.10351
73 -> 80 0.20408
74 -> 80 -0.23159
75 -> 80 0.51753
79 -> 82 -0.28353

Excited State 11: Singlet-A 4.8011 eV 258.24 nm f=0.4474 <S**2>=0.000
75 -> 80 -0.13546
77 -> 81 0.32590
78 -> 81 -0.21175
78 -> 83 0.14427
78 -> 84 -0.15086
79 -> 81 0.11002
79 -> 82 -0.14023
79 -> 83 0.45852

Excited State 12: Singlet-A 5.0279 eV 246.59 nm f=0.0275 <S**2>=0.000
74 -> 80 -0.34117
75 -> 80 -0.16593
77 -> 81 0.34886
78 -> 83 0.26142
79 -> 83 -0.30099
79 -> 84 -0.18053
79 -> 86 0.10714

Excited State 13: Singlet-A 5.0431 eV 245.85 nm f=0.0359 <S**2>=0.000
74 -> 80 0.47168
75 -> 80 0.27381
77 -> 81 0.22437
79 -> 83 -0.18189
79 -> 84 -0.27426

Excited State 14: Singlet-A 5.0995 eV 243.13 nm f=0.0016 <S**2>=0.000
78 -> 82 0.54387
78 -> 83 0.11386
79 -> 82 0.15479
79 -> 83 -0.10580
79 -> 84 0.14248
79 -> 85 0.32020

Excited State 15: Singlet-A 5.1161 eV 242.34 nm f=0.0175 <S**2>=0.000
78 -> 82 -0.35670
79 -> 82 -0.13189
79 -> 85 0.55473
79 -> 88 0.11878

Excited State 16: Singlet-A 5.2064 eV 238.14 nm f=0.0671 <S**2>=0.000
74 -> 80 0.14148
78 -> 82 -0.14098
78 -> 83 0.32949
79 -> 83 -0.13332
79 -> 84 0.48776
79 -> 85 -0.15736
79 -> 86 0.17061

Excited State 17: Singlet-A 5.3229 eV 232.93 nm f=0.0353 <S**2>=0.000
78 -> 83 -0.12038
78 -> 84 0.13290
78 -> 86 0.16895
79 -> 84 -0.14105
79 -> 86 0.61058

Excited State 18: Singlet-A 5.3642 eV 231.13 nm f=0.0053 <S**2>=0.000
78 -> 84 0.15211
78 -> 85 0.47055
78 -> 87 -0.16426
79 -> 87 -0.44814

Excited State 19: Singlet-A 5.4181 eV 228.83 nm f=0.0601 <S**2>=0.000
78 -> 83 0.14699
78 -> 84 0.61056
78 -> 85 -0.12453
79 -> 83 0.10388
79 -> 86 -0.14988

Excited State 20: Singlet-A 5.5029 eV 225.31 nm f=0.4192 <S**2>=0.000
75 -> 81 0.23250
77 -> 81 -0.33396
78 -> 83 0.34259
78 -> 86 -0.29265
79 -> 84 -0.20409
79 -> 86 0.10351

Excited State 21: Singlet-A 5.5182 eV 224.68 nm f=0.0022 <S**2>=0.000
78 -> 85 0.42945
78 -> 89 0.10726
79 -> 87 0.42802
79 -> 88 0.30259

Excited State 22: Singlet-A 5.5613 eV 222.94 nm f=0.0037 <S**2>=0.000
72 -> 80 0.10852
78 -> 85 -0.15356
78 -> 87 0.16197
79 -> 85 -0.11445
79 -> 87 -0.25900
79 -> 88 0.56989

Excited State 23: Singlet-A 5.5681 eV 222.67 nm f=0.0555 <S**2>=0.000
72 -> 80 0.56961
78 -> 86 0.30316
79 -> 86 -0.10154
79 -> 88 -0.10807

Excited State 24: Singlet-A 5.6049 eV 221.21 nm f=0.2283 <S**2>=0.000
72 -> 80 -0.30110
74 -> 81 -0.15116
76 -> 81 0.12768
77 -> 81 -0.13390
77 -> 82 -0.17997
78 -> 83 0.12347
78 -> 84 -0.11860
78 -> 86 0.44543
79 -> 84 -0.14678
79 -> 86 -0.10179

Excited State 25: Singlet-A 5.6398 eV 219.84 nm f=0.0948 <S**2>=0.000
76 -> 81 0.47086
76 -> 84 0.12939
77 -> 82 -0.40432
78 -> 86 -0.11480

Excited State 26: Singlet-A 5.6960 eV 217.67 nm f=0.0024 <S**2>=0.000
78 -> 87 0.52825
78 -> 89 0.10344
79 -> 88 -0.11780
79 -> 89 0.37774

Excited State 27: Singlet-A 5.7819 eV 214.44 nm f=0.0009 <S**2>=0.000
78 -> 87 -0.23862
78 -> 88 -0.40342
79 -> 85 -0.10065
79 -> 89 0.44605
79 -> 90 0.17301

Excited State 28: Singlet-A 5.7883 eV 214.20 nm f=0.0033 <S**2>=0.000
71 -> 80 -0.20436
76 -> 81 0.48269
77 -> 82 0.43083

Excited State 29: Singlet-A 5.8624 eV 211.49 nm f=0.0050 <S**2>=0.000
78 -> 87 -0.21038
78 -> 88 0.37382

78 -> 89 -0.26787
79 -> 89 0.33490
79 -> 90 -0.31955

Excited State 30: Singlet-A 5.9636 eV 207.90 nm f=0.0875 <S**2>=0.000
71 -> 80 0.64852
76 -> 81 0.11760
77 -> 82 0.14868

Single-point TDDFT PBE0/6-311++G(2df,2p)/PCM(DMSO) over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometry

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0222 eV 410.25 nm f=0.3331 <S**2>=0.000
79 -> 80 0.69812
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.35003078
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4101 eV 363.57 nm f=0.4566 <S**2>=0.000
78 -> 80 0.69114

Excited State 3: Singlet-A 3.9026 eV 317.70 nm f=0.0000 <S**2>=0.000
73 -> 80 -0.31871
74 -> 80 0.61088

Excited State 4: Singlet-A 4.1249 eV 300.58 nm f=0.2144 <S**2>=0.000
77 -> 80 -0.11637
78 -> 83 -0.11730
79 -> 81 0.67161

Excited State 5: Singlet-A 4.2782 eV 289.80 nm f=0.0846 <S**2>=0.000
76 -> 80 0.15931
77 -> 80 0.57758
78 -> 81 0.24395
79 -> 83 0.23497

Excited State 6: Singlet-A 4.3252 eV 286.65 nm f=0.0616 <S**2>=0.000
76 -> 80 -0.38707
77 -> 80 -0.17707
78 -> 81 0.43853
78 -> 82 0.10599
79 -> 81 -0.10018
79 -> 82 0.15927
79 -> 83 0.21894

Excited State 7: Singlet-A 4.3373 eV 285.86 nm f=0.0921 <S**2>=0.000
76 -> 80 0.49585
77 -> 80 -0.30590
77 -> 82 -0.10024
78 -> 81 0.30359
78 -> 82 -0.10358
79 -> 81 -0.10169
79 -> 82 -0.10220

Excited State 8: Singlet-A 4.5285 eV 273.78 nm f=0.0004 <S**2>=0.000
70 -> 80 0.66966
73 -> 80 0.14586

Excited State 9: Singlet-A 4.7173 eV 262.83 nm f=0.0706 <S**2>=0.000
76 -> 80 0.21359
78 -> 81 -0.11404
78 -> 82 0.16278
79 -> 82 0.63320

Excited State 10: Singlet-A 4.9804 eV 248.95 nm f=0.7557 <S**2>=0.000
75 -> 80 -0.15754
77 -> 81 -0.22589
78 -> 81 -0.32077
78 -> 84 0.12483
79 -> 82 -0.10123
79 -> 83 0.52125

Excited State 11: Singlet-A 5.0958 eV 243.31 nm f=0.0680 <S**2>=0.000
75 -> 80 0.66140
79 -> 83 0.12546
79 -> 86 -0.10046

Excited State 12: Singlet-A 5.1373 eV 241.34 nm f=0.0944 <S**2>=0.000
76 -> 80 0.10747
78 -> 82 0.64322
79 -> 82 -0.20906

Excited State 13: Singlet-A 5.3077 eV 233.59 nm f=0.0002 <S**2>=0.000
70 -> 80 -0.15567
73 -> 80 0.59383
74 -> 80 0.31209

Excited State 14: Singlet-A 5.3427 eV 232.06 nm f=0.0029 <S**2>=0.000
75 -> 80 -0.10796
75 -> 81 -0.13627
77 -> 81 0.27504
79 -> 83 0.13836
79 -> 84 0.50445
79 -> 86 -0.30235

Excited State 15: Singlet-A 5.4350 eV 228.12 nm f=0.0000 <S**2>=0.000
79 -> 85 0.62778
79 -> 87 -0.25619
79 -> 89 0.13690

Excited State 16: Singlet-A 5.4556 eV 227.26 nm f=0.0577 <S**2>=0.000
77 -> 81 0.36132
78 -> 83 0.44402
79 -> 83 0.16586
79 -> 86 0.33006

Excited State 17: Singlet-A 5.5729 eV 222.48 nm f=0.0131 <S**2>=0.000
78 -> 83 -0.35268
79 -> 84 0.33197
79 -> 86 0.48053

Excited State 18: Singlet-A 5.6661 eV 218.82 nm f=0.0006 <S**2>=0.000

78 -> 85 0.26632
79 -> 85 0.19990
79 -> 87 0.58273
79 -> 89 0.14110

Excited State 19: Singlet-A 5.7642 eV 215.09 nm f=0.0613 <S**2>=0.000
72 -> 80 0.23871
75 -> 83 0.13562
77 -> 81 0.17952
78 -> 84 0.53100
78 -> 86 -0.25746

Excited State 20: Singlet-A 5.7974 eV 213.86 nm f=0.3739 <S**2>=0.000
72 -> 80 0.33209
77 -> 81 0.31345
77 -> 82 -0.16994
78 -> 83 -0.31070
78 -> 84 -0.22423
78 -> 86 0.10610
79 -> 83 0.13215
79 -> 84 -0.21802

Excited State 21: Singlet-A 5.8286 eV 212.72 nm f=0.1848 <S**2>=0.000
72 -> 80 0.52981
77 -> 81 -0.18845
77 -> 82 0.21665
78 -> 83 0.16997
78 -> 86 0.15809
79 -> 84 0.12114
79 -> 86 0.10649

Excited State 22: Singlet-A 5.8649 eV 211.40 nm f=0.0002 <S**2>=0.000
78 -> 85 -0.23896
79 -> 88 0.61081
79 -> 89 -0.11706
79 -> 90 0.17899

Excited State 23: Singlet-A 5.8929 eV 210.40 nm f=0.0012 <S**2>=0.000
78 -> 85 0.54546
78 -> 89 0.13053
79 -> 87 -0.21455
79 -> 88 0.18946
79 -> 89 -0.26133

Excited State 24: Singlet-A 5.9138 eV 209.65 nm f=0.1607 <S**2>=0.000
71 -> 80 -0.14700
76 -> 81 0.30776
76 -> 84 -0.12090
77 -> 81 0.20305
77 -> 82 0.47552
78 -> 82 -0.14927
78 -> 83 -0.11719
79 -> 84 -0.13725

Excited State 25: Singlet-A 5.9761 eV 207.47 nm f=0.1175 <S**2>=0.000
72 -> 80 -0.12810
75 -> 81 -0.30590
76 -> 81 -0.13670
78 -> 84 0.30150

78 -> 86 0.46147
79 -> 84 -0.11684

Excited State 26: Singlet-A 6.0302 eV 205.60 nm f=0.0017 <S**2>=0.000
78 -> 87 -0.38526
79 -> 85 -0.14679
79 -> 87 -0.15619
79 -> 88 0.13993
79 -> 89 0.47892
79 -> 91 -0.10491

Excited State 27: Singlet-A 6.0523 eV 204.85 nm f=0.0186 <S**2>=0.000
71 -> 80 0.42258
75 -> 81 0.27992
76 -> 81 0.35329
78 -> 84 0.11130
78 -> 86 0.25976

Excited State 28: Singlet-A 6.0817 eV 203.87 nm f=0.0567 <S**2>=0.000
71 -> 80 -0.43537
75 -> 81 0.45486
78 -> 86 0.21220

Excited State 29: Singlet-A 6.1365 eV 202.04 nm f=0.0025 <S**2>=0.000
78 -> 87 -0.34561
78 -> 88 -0.27326
79 -> 85 0.12726
79 -> 88 -0.17803
79 -> 89 -0.23938
79 -> 90 0.41274

Excited State 30: Singlet-A 6.1761 eV 200.75 nm f=0.0001 <S**2>=0.000
66 -> 80 -0.10964
73 -> 81 0.56810
74 -> 81 0.33042

1-

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.6233 eV 472.62 nm f=1.0701 <S**2>=0.000
79 -> 80 0.70443
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1042.89580046
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2513 eV 381.34 nm f=0.1688 <S**2>=0.000
78 -> 80 0.69694

Excited State 3: Singlet-A 3.7368 eV 331.79 nm f=0.2271 <S**2>=0.000
77 -> 80 -0.12778
78 -> 83 -0.10110
79 -> 81 0.67121

Excited State 4: Singlet-A 3.8312 eV 323.62 nm f=0.0000 <S**2>=0.000
72 -> 80 0.62028
72 -> 81 0.10337
73 -> 80 -0.15407
76 -> 80 -0.25871

Excited State 5: Singlet-A 4.0578 eV 305.55 nm f=0.0717 <S**2>=0.000
77 -> 80 0.64801
78 -> 83 -0.10544
79 -> 83 0.17784

Excited State 6: Singlet-A 4.1478 eV 298.92 nm f=0.0071 <S**2>=0.000
75 -> 80 -0.46090
79 -> 82 0.50862

Excited State 7: Singlet-A 4.2000 eV 295.20 nm f=0.0002 <S**2>=0.000
72 -> 80 0.25023
76 -> 80 0.64734

Excited State 8: Singlet-A 4.2653 eV 290.68 nm f=0.0222 <S**2>=0.000
75 -> 80 0.22920
77 -> 80 -0.17638
78 -> 81 0.55106
79 -> 82 0.15637
79 -> 83 0.25226

Excited State 9: Singlet-A 4.3420 eV 285.55 nm f=0.0584 <S**2>=0.000
75 -> 80 0.46235
78 -> 81 -0.23023
79 -> 82 0.43519
79 -> 83 -0.17603

Excited State 10: Singlet-A 4.5804 eV 270.68 nm f=0.0003 <S**2>=0.000
69 -> 80 0.65045
69 -> 81 0.10576
73 -> 80 -0.21676

Excited State 11: Singlet-A 4.6271 eV 267.95 nm f=0.4263 <S**2>=0.000
77 -> 80 -0.13611
77 -> 81 -0.12142
78 -> 81 -0.31785
79 -> 83 0.55325
79 -> 85 0.13925

Excited State 12: Singlet-A 4.7485 eV 261.10 nm f=0.0008 <S**2>=0.000
79 -> 84 0.66151
79 -> 86 0.16398
79 -> 89 -0.13662

Excited State 13: Singlet-A 4.8469 eV 255.80 nm f=0.0004 <S**2>=0.000
69 -> 80 0.21898
72 -> 80 0.14607
73 -> 80 0.64133

Excited State 14: Singlet-A 4.9223 eV 251.88 nm f=0.0049 <S**2>=0.000
74 -> 80 0.27063
77 -> 81 0.10462
78 -> 81 0.11022
79 -> 85 0.60552

Excited State 15: Singlet-A 4.9453 eV 250.71 nm f=0.0399 <S**2>=0.000
77 -> 81 0.42755
78 -> 82 0.24294
78 -> 83 0.38870

79 -> 81 0.10647
79 -> 83 0.21543

Excited State 16: Singlet-A 5.0192 eV 247.02 nm f=0.0046 <S**2>=0.000
78 -> 84 0.14915
79 -> 84 -0.13825
79 -> 86 0.65290
79 -> 89 0.10829

Excited State 17: Singlet-A 5.0864 eV 243.76 nm f=0.0304 <S**2>=0.000
74 -> 80 0.62584
77 -> 81 -0.11870
79 -> 85 -0.23310
79 -> 88 0.12698

Excited State 18: Singlet-A 5.1990 eV 238.48 nm f=0.0847 <S**2>=0.000
77 -> 81 0.12143
78 -> 82 -0.11790
78 -> 85 0.11821
79 -> 85 0.11781
79 -> 88 0.63383

Excited State 19: Singlet-A 5.2122 eV 237.87 nm f=0.0010 <S**2>=0.000
79 -> 87 0.67410
79 -> 90 0.13178

Excited State 20: Singlet-A 5.2403 eV 236.60 nm f=0.0556 <S**2>=0.000
77 -> 81 -0.11422
78 -> 82 0.62111
78 -> 83 -0.21952
78 -> 85 0.13192

Excited State 21: Singlet-A 5.2945 eV 234.18 nm f=0.0002 <S**2>=0.000
78 -> 86 0.13964
79 -> 84 0.15176
79 -> 89 0.65050

Excited State 22: Singlet-A 5.4068 eV 229.31 nm f=0.0008 <S**2>=0.000
78 -> 84 0.60334
78 -> 86 -0.24448
78 -> 89 -0.12643
79 -> 86 -0.14085

Excited State 23: Singlet-A 5.4515 eV 227.43 nm f=0.0038 <S**2>=0.000
71 -> 80 -0.12517
74 -> 81 0.10294
78 -> 83 0.20528
78 -> 85 0.58772
78 -> 88 -0.20753
79 -> 88 -0.10887

Excited State 24: Singlet-A 5.4933 eV 225.70 nm f=0.0000 <S**2>=0.000
78 -> 87 0.14888
79 -> 87 -0.12540
79 -> 90 0.66434

Excited State 25: Singlet-A 5.5482 eV 223.47 nm f=0.1106 <S**2>=0.000
71 -> 80 0.61658
77 -> 81 0.21915

78 -> 83 -0.11282
78 -> 85 0.17232

Excited State 26: Singlet-A 5.6099 eV 221.01 nm f=0.0003 <S**2>=0.000
76 -> 81 0.67452
76 -> 82 -0.11044

Excited State 27: Singlet-A 5.6714 eV 218.61 nm f=0.8259 <S**2>=0.000
71 -> 80 0.24688
77 -> 81 -0.40393
77 -> 82 0.11028
78 -> 83 0.41500
79 -> 88 0.16347

Excited State 28: Singlet-A 5.6949 eV 217.71 nm f=0.0003 <S**2>=0.000
78 -> 84 0.15913
78 -> 86 0.54984
78 -> 89 -0.30414
79 -> 91 0.20433

Excited State 29: Singlet-A 5.7979 eV 213.84 nm f=0.0002 <S**2>=0.000
78 -> 86 -0.13227
78 -> 87 0.40994
79 -> 91 0.47495
79 -> 93 -0.17387

Excited State 30: Singlet-A 5.8156 eV 213.19 nm f=0.0000 <S**2>=0.000
78 -> 84 0.16228
78 -> 86 0.17627
78 -> 87 0.48827
78 -> 89 0.10096
78 -> 90 -0.12144
79 -> 90 -0.10802
79 -> 91 -0.36882

1’

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9668 eV 417.90 nm f=0.4940 <S**2>=0.000
79 -> 80 0.70214
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.34937717
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4245 eV 362.06 nm f=0.3454 <S**2>=0.000
78 -> 80 0.69416

Excited State 3: Singlet-A 3.8999 eV 317.91 nm f=0.0000 <S**2>=0.000
74 -> 80 0.68803
74 -> 81 0.10168

Excited State 4: Singlet-A 4.0567 eV 305.63 nm f=0.2172 <S**2>=0.000
78 -> 83 -0.11353
79 -> 81 0.67742

Excited State 5: Singlet-A 4.2721 eV 290.22 nm f=0.1553 <S**2>=0.000
76 -> 80 -0.10398
77 -> 80 0.63373

78 -> 81 0.14115
79 -> 83 0.20118

Excited State 6: Singlet-A 4.3365 eV 285.91 nm f=0.0111 <S**2>=0.000
76 -> 80 0.60742
77 -> 80 0.13676
77 -> 82 0.11589
78 -> 82 0.14563
79 -> 82 0.25007

Excited State 7: Singlet-A 4.3476 eV 285.18 nm f=0.0339 <S**2>=0.000
76 -> 80 0.10220
77 -> 80 -0.21277
77 -> 81 -0.10041
78 -> 81 0.55500
79 -> 81 -0.11333
79 -> 83 0.28831
79 -> 84 -0.11585

Excited State 8: Singlet-A 4.5330 eV 273.52 nm f=0.0004 <S**2>=0.000
70 -> 80 0.68808

Excited State 9: Singlet-A 4.6508 eV 266.59 nm f=0.0157 <S**2>=0.000
76 -> 80 -0.28787
78 -> 82 0.11023
79 -> 82 0.62515

Excited State 10: Singlet-A 4.9198 eV 252.01 nm f=0.7995 <S**2>=0.000
77 -> 80 -0.10313
77 -> 81 -0.20799
78 -> 81 -0.35767
78 -> 84 0.11491
79 -> 83 0.51861

Excited State 11: Singlet-A 5.0956 eV 243.31 nm f=0.0203 <S**2>=0.000
75 -> 80 0.66857
79 -> 84 0.11508
79 -> 86 -0.12483

Excited State 12: Singlet-A 5.1419 eV 241.13 nm f=0.0449 <S**2>=0.000
76 -> 80 -0.10227
78 -> 82 0.63879
79 -> 82 -0.16038
79 -> 83 -0.11348
79 -> 84 -0.13370

Excited State 13: Singlet-A 5.2999 eV 233.94 nm f=0.0041 <S**2>=0.000
75 -> 80 -0.15302
75 -> 81 -0.11409
77 -> 81 0.33479
78 -> 82 0.15621
79 -> 83 0.14117
79 -> 84 0.46575
79 -> 86 -0.23656

Excited State 14: Singlet-A 5.3451 eV 231.96 nm f=0.0003 <S**2>=0.000
79 -> 85 0.65183
79 -> 87 -0.16112
79 -> 88 -0.10981

79 -> 89 -0.13061

Excited State 15: Singlet-A 5.4067 eV 229.32 nm f=0.0268 <S**2>=0.000
77 -> 81 0.33412
78 -> 83 0.38324
79 -> 83 0.15348
79 -> 86 0.41777

Excited State 16: Singlet-A 5.4672 eV 226.78 nm f=0.0002 <S**2>=0.000
73 -> 80 0.68479
73 -> 81 -0.14182

Excited State 17: Singlet-A 5.5411 eV 223.75 nm f=0.0351 <S**2>=0.000
78 -> 83 -0.38028
79 -> 84 0.34007
79 -> 86 0.45317

Excited State 18: Singlet-A 5.5913 eV 221.75 nm f=0.0011 <S**2>=0.000
78 -> 85 0.20949
79 -> 85 0.11721
79 -> 87 0.63453

Excited State 19: Singlet-A 5.7745 eV 214.71 nm f=0.1239 <S**2>=0.000
72 -> 80 0.31741
75 -> 83 0.12277
77 -> 81 0.23449
77 -> 82 -0.17624
78 -> 84 0.44314
78 -> 86 -0.22376

Excited State 20: Singlet-A 5.7858 eV 214.29 nm f=0.3706 <S**2>=0.000
72 -> 80 -0.23164
77 -> 81 -0.26046
77 -> 82 0.13702
78 -> 83 0.33258
78 -> 84 0.33139
78 -> 86 -0.15464
79 -> 83 -0.11598
79 -> 84 0.23875

Excited State 21: Singlet-A 5.8158 eV 213.18 nm f=0.0000 <S**2>=0.000
79 -> 85 0.11345
79 -> 88 0.65518
79 -> 90 -0.18912

Excited State 22: Singlet-A 5.8302 eV 212.66 nm f=0.1372 <S**2>=0.000
72 -> 80 0.54030
77 -> 81 -0.15804
77 -> 82 0.25417
78 -> 83 0.12696
78 -> 86 0.13287
79 -> 84 0.12058
79 -> 86 0.10162

Excited State 23: Singlet-A 5.8928 eV 210.40 nm f=0.0005 <S**2>=0.000
78 -> 85 0.59660
78 -> 89 -0.13906
79 -> 87 -0.17162
79 -> 89 0.24616

Excited State 24: Singlet-A 5.9124 eV 209.70 nm f=0.2229 <S**2>=0.000
71 -> 80 -0.14678
72 -> 80 -0.10875
76 -> 81 -0.27884
76 -> 84 0.10236
77 -> 81 0.20999
77 -> 82 0.45145
78 -> 82 -0.12593
78 -> 83 -0.18036
78 -> 84 0.10908
78 -> 86 -0.11320
79 -> 84 -0.12741

Excited State 25: Singlet-A 5.9943 eV 206.84 nm f=0.0016 <S**2>=0.000
78 -> 85 -0.17745
78 -> 87 0.30462
79 -> 85 0.13234
79 -> 87 0.12667
79 -> 89 0.53888
79 -> 91 -0.10338

Excited State 26: Singlet-A 5.9944 eV 206.83 nm f=0.1191 <S**2>=0.000
72 -> 80 -0.10721
75 -> 81 -0.37179
78 -> 84 0.31078
78 -> 86 0.44073

Excited State 27: Singlet-A 6.0565 eV 204.71 nm f=0.0847 <S**2>=0.000
71 -> 80 0.60990
76 -> 81 -0.32097

Excited State 28: Singlet-A 6.0884 eV 203.64 nm f=0.0018 <S**2>=0.000
78 -> 88 0.21793
79 -> 88 0.17166
79 -> 89 0.13808
79 -> 90 0.60079

Excited State 29: Singlet-A 6.1147 eV 202.76 nm f=0.0176 <S**2>=0.000
75 -> 81 0.53787
78 -> 84 0.13763
78 -> 86 0.36502
79 -> 92 0.10477

Excited State 30: Singlet-A 6.1773 eV 200.71 nm f=0.0401 <S**2>=0.000
71 -> 80 0.27576
76 -> 81 0.54108
77 -> 82 0.31888

1'-

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5969 eV 477.44 nm f=1.1123 <S**2>=0.000
79 -> 80 0.70384
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1042.89345566
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2716 eV 378.97 nm f=0.1088 <S**2>=0.000
78 -> 80 0.68902
79 -> 81 -0.13338

Excited State 3: Singlet-A 3.6717 eV 337.68 nm f=0.2148 <S**2>=0.000
77 -> 80 0.23665
78 -> 80 0.13420
79 -> 81 0.63376

Excited State 4: Singlet-A 3.8204 eV 324.53 nm f=0.0119 <S**2>=0.000
72 -> 80 0.53421
74 -> 80 0.13311
75 -> 80 -0.14280
76 -> 80 -0.18517
77 -> 80 0.29057
79 -> 81 -0.16849

Excited State 5: Singlet-A 3.9107 eV 317.03 nm f=0.0507 <S**2>=0.000
72 -> 80 -0.36683
77 -> 80 0.54873
79 -> 81 -0.15247
79 -> 83 0.12322

Excited State 6: Singlet-A 4.1293 eV 300.26 nm f=0.0010 <S**2>=0.000
75 -> 80 0.27029
76 -> 80 -0.21871
79 -> 82 0.59807

Excited State 7: Singlet-A 4.2512 eV 291.64 nm f=0.0264 <S**2>=0.000
76 -> 80 0.20094
77 -> 81 0.10304
78 -> 81 0.46594
79 -> 83 0.43653

Excited State 8: Singlet-A 4.3242 eV 286.72 nm f=0.0115 <S**2>=0.000
75 -> 80 -0.39591
76 -> 80 0.43485
78 -> 81 -0.16854
79 -> 82 0.33319

Excited State 9: Singlet-A 4.4161 eV 280.76 nm f=0.0317 <S**2>=0.000
72 -> 80 0.17124
74 -> 80 -0.10465
75 -> 80 0.45647
76 -> 80 0.34545
77 -> 80 0.14320
78 -> 81 -0.26921

Excited State 10: Singlet-A 4.5767 eV 270.90 nm f=0.3855 <S**2>=0.000
69 -> 80 -0.10800
75 -> 80 -0.10727
76 -> 80 -0.17071
77 -> 80 -0.14893
78 -> 81 -0.36027
79 -> 83 0.46806
79 -> 84 0.13427
79 -> 85 0.14091

Excited State 11: Singlet-A 4.5984 eV 269.63 nm f=0.0098 <S**2>=0.000

69 -> 80 0.67752
69 -> 81 -0.10760

Excited State 12: Singlet-A 4.6792 eV 264.97 nm f=0.0219 <S**2>=0.000
79 -> 84 0.65522
79 -> 86 0.11521
79 -> 89 -0.11646

Excited State 13: Singlet-A 4.8727 eV 254.45 nm f=0.0194 <S**2>=0.000
74 -> 80 -0.17602
77 -> 81 -0.21604
78 -> 81 0.13919
79 -> 85 0.54022
79 -> 86 -0.24745

Excited State 14: Singlet-A 4.9102 eV 252.50 nm f=0.0064 <S**2>=0.000
77 -> 81 0.46525
78 -> 83 0.36409
79 -> 83 -0.17470
79 -> 85 0.12840
79 -> 86 -0.12762
79 -> 87 0.16369
79 -> 88 0.15327

Excited State 15: Singlet-A 4.9615 eV 249.89 nm f=0.0038 <S**2>=0.000
78 -> 84 -0.13512
79 -> 85 0.29758
79 -> 86 0.58881
79 -> 89 0.10308

Excited State 16: Singlet-A 4.9804 eV 248.94 nm f=0.0005 <S**2>=0.000
73 -> 80 0.68548
73 -> 81 0.10122

Excited State 17: Singlet-A 5.1004 eV 243.09 nm f=0.0267 <S**2>=0.000
74 -> 80 0.37679
78 -> 83 -0.13343
79 -> 87 0.49776
79 -> 88 0.17002

Excited State 18: Singlet-A 5.1408 eV 241.18 nm f=0.0083 <S**2>=0.000
74 -> 80 0.47010
79 -> 85 0.17121
79 -> 87 -0.37818
79 -> 88 0.16862

Excited State 19: Singlet-A 5.1835 eV 239.19 nm f=0.0504 <S**2>=0.000
74 -> 80 -0.19975
78 -> 82 -0.12153
78 -> 83 -0.14085
79 -> 84 -0.11522
79 -> 86 0.10109
79 -> 88 0.57315
79 -> 89 -0.13162
79 -> 90 0.10870

Excited State 20: Singlet-A 5.2222 eV 237.42 nm f=0.0214 <S**2>=0.000
78 -> 82 0.65386

Excited State 21: Singlet-A 5.2576 eV 235.82 nm f=0.0079 <S**2>=0.000
78 -> 86 -0.11800
79 -> 87 -0.17103
79 -> 88 0.13859
79 -> 89 0.62465

Excited State 22: Singlet-A 5.4208 eV 228.72 nm f=0.4416 <S**2>=0.000
71 -> 80 0.14529
75 -> 81 0.17024
76 -> 81 0.22019
77 -> 81 -0.32256
78 -> 83 0.36853
78 -> 84 0.19941
79 -> 90 0.20973

Excited State 23: Singlet-A 5.4268 eV 228.47 nm f=0.0451 <S**2>=0.000
77 -> 81 0.10745
78 -> 83 -0.11351
79 -> 88 -0.12623
79 -> 90 0.62244

Excited State 24: Singlet-A 5.4383 eV 227.98 nm f=0.0797 <S**2>=0.000
76 -> 81 -0.12051
77 -> 81 0.13611
78 -> 83 -0.10174
78 -> 84 0.58253
78 -> 86 -0.17077
78 -> 89 -0.11887

Excited State 25: Singlet-A 5.4913 eV 225.78 nm f=0.0076 <S**2>=0.000
76 -> 81 -0.11867
78 -> 83 0.10515
78 -> 85 0.55704
78 -> 86 -0.23628
78 -> 87 0.11996
78 -> 88 0.14027

Excited State 26: Singlet-A 5.5989 eV 221.45 nm f=0.0096 <S**2>=0.000
71 -> 80 0.64166
76 -> 81 -0.12061

Excited State 27: Singlet-A 5.6734 eV 218.54 nm f=0.0179 <S**2>=0.000
70 -> 80 0.12348
75 -> 81 0.14853
75 -> 82 -0.10435
76 -> 82 -0.17873
77 -> 82 0.58352
78 -> 82 0.13185
78 -> 86 0.10295

Excited State 28: Singlet-A 5.6958 eV 217.68 nm f=0.0046 <S**2>=0.000
77 -> 82 -0.10320
78 -> 85 0.18476
78 -> 86 0.41840
78 -> 89 -0.22549
79 -> 91 0.40083

Excited State 29: Singlet-A 5.7433 eV 215.88 nm f=0.0304 <S**2>=0.000
78 -> 84 -0.14678

78 -> 85 -0.15777
78 -> 86 -0.34507
78 -> 87 -0.12620
79 -> 91 0.39640
79 -> 92 0.18872
79 -> 93 0.18961
79 -> 94 -0.16539

Excited State 30: Singlet-A 5.7982 eV 213.83 nm f=0.1250 <S**2>=0.000
75 -> 81 0.15168
76 -> 81 0.24336
78 -> 83 -0.15570
78 -> 86 -0.10430
78 -> 87 0.19014
79 -> 91 0.32269
79 -> 92 -0.29980
79 -> 93 -0.16653
79 -> 94 0.25797

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1067 eV 399.09 nm f=0.4734 <S**2>=0.000
78 -> 80 0.17305
79 -> 80 0.67914
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.33995191
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4113 eV 363.46 nm f=0.1406 <S**2>=0.000
78 -> 80 0.67931
79 -> 80 -0.17978

Excited State 3: Singlet-A 3.8903 eV 318.70 nm f=0.0264 <S**2>=0.000
73 -> 80 0.63783
73 -> 84 -0.10825
74 -> 80 0.16237
75 -> 80 -0.14859
77 -> 80 0.13942

Excited State 4: Singlet-A 4.0338 eV 307.36 nm f=0.3401 <S**2>=0.000
73 -> 80 -0.16278
77 -> 80 0.63512
79 -> 81 0.21633

Excited State 5: Singlet-A 4.1835 eV 296.36 nm f=0.1393 <S**2>=0.000
77 -> 80 -0.22176
78 -> 81 0.16688
78 -> 83 -0.20048
79 -> 81 0.58118
79 -> 83 0.15249

Excited State 6: Singlet-A 4.2796 eV 289.71 nm f=0.0154 <S**2>=0.000
76 -> 80 0.66215
77 -> 82 -0.12347
78 -> 82 -0.10401
79 -> 82 -0.15395

Excited State 7: Singlet-A 4.3670 eV 283.91 nm f=0.0595 <S**2>=0.000
78 -> 81 0.61029
79 -> 81 -0.24591
79 -> 83 0.22365

Excited State 8: Singlet-A 4.5368 eV 273.29 nm f=0.0005 <S**2>=0.000
71 -> 80 0.68581
71 -> 84 -0.10988

Excited State 9: Singlet-A 4.7742 eV 259.69 nm f=0.0164 <S**2>=0.000
76 -> 80 0.19200
78 -> 82 0.23854
79 -> 82 0.62083

Excited State 10: Singlet-A 4.9263 eV 251.68 nm f=0.4361 <S**2>=0.000
74 -> 80 0.12306
75 -> 80 -0.32911
77 -> 81 -0.30191
78 -> 81 -0.21845
78 -> 83 -0.17394
78 -> 84 -0.13192
79 -> 81 -0.13141
79 -> 83 0.35530
79 -> 84 -0.12301

Excited State 11: Singlet-A 5.0102 eV 247.47 nm f=0.1116 <S**2>=0.000
70 -> 80 0.10572
73 -> 80 0.14716
74 -> 80 -0.22267
75 -> 80 0.49831
77 -> 80 0.10917
77 -> 81 -0.26693
78 -> 81 -0.11103
79 -> 83 0.19578

Excited State 12: Singlet-A 5.2027 eV 238.31 nm f=0.0037 <S**2>=0.000
78 -> 82 0.63243
79 -> 82 -0.26731

Excited State 13: Singlet-A 5.2581 eV 235.80 nm f=0.1852 <S**2>=0.000
74 -> 80 -0.19953
77 -> 81 0.37284
78 -> 83 0.27451
79 -> 83 0.38075
79 -> 84 -0.24095

Excited State 14: Singlet-A 5.3086 eV 233.55 nm f=0.0698 <S**2>=0.000
74 -> 80 0.51266
75 -> 80 0.28863
77 -> 81 0.15760
78 -> 84 -0.10310
79 -> 84 -0.27007
79 -> 86 -0.12401

Excited State 15: Singlet-A 5.3827 eV 230.34 nm f=0.0488 <S**2>=0.000
74 -> 80 0.27153
78 -> 81 -0.10134
78 -> 83 0.31369
79 -> 83 0.24249

79 -> 84 0.46226

Excited State 16: Singlet-A 5.4773 eV 226.36 nm f=0.0030 <S**2>=0.000
79 -> 85 0.66911
79 -> 89 -0.14102

Excited State 17: Singlet-A 5.5069 eV 225.14 nm f=0.0075 <S**2>=0.000
74 -> 81 -0.11574
78 -> 84 -0.22142
78 -> 86 -0.19504
79 -> 86 0.59297

Excited State 18: Singlet-A 5.5502 eV 223.39 nm f=0.6796 <S**2>=0.000
75 -> 81 0.20491
77 -> 81 -0.35515
78 -> 83 0.37279
78 -> 84 0.12167
78 -> 86 0.18387
79 -> 84 -0.27679

Excited State 19: Singlet-A 5.6434 eV 219.70 nm f=0.0164 <S**2>=0.000
75 -> 82 -0.10839
76 -> 81 -0.10525
76 -> 84 -0.14523
77 -> 82 0.55209
78 -> 82 -0.10105
78 -> 83 0.10968
78 -> 84 -0.27237
79 -> 86 -0.11854

Excited State 20: Singlet-A 5.6474 eV 219.54 nm f=0.0281 <S**2>=0.000
77 -> 82 0.29497
78 -> 83 -0.18959
78 -> 84 0.51027
79 -> 86 0.19328

Excited State 21: Singlet-A 5.6995 eV 217.53 nm f=0.0021 <S**2>=0.000
78 -> 85 0.52803
78 -> 87 -0.21151
79 -> 87 0.38463

Excited State 22: Singlet-A 5.7505 eV 215.61 nm f=0.1408 <S**2>=0.000
74 -> 81 0.12384
78 -> 84 -0.18463
78 -> 86 0.58698
79 -> 84 0.15404
79 -> 86 0.16129

Excited State 23: Singlet-A 5.8735 eV 211.09 nm f=0.0028 <S**2>=0.000
78 -> 85 -0.38181
78 -> 89 0.16386
79 -> 87 0.53388
79 -> 89 -0.10311

Excited State 24: Singlet-A 5.8893 eV 210.52 nm f=0.0083 <S**2>=0.000
68 -> 80 0.10129
70 -> 80 0.63622
77 -> 84 -0.13877

Excited State 25: Singlet-A 6.0094 eV 206.32 nm f=0.0095 <S**2>=0.000
72 -> 80 -0.23470
76 -> 81 0.63688

Excited State 26: Singlet-A 6.0145 eV 206.14 nm f=0.0018 <S**2>=0.000
77 -> 85 0.14197
78 -> 85 0.10106
78 -> 87 0.57102
79 -> 87 0.16283
79 -> 88 0.15783
79 -> 89 0.22837

Excited State 27: Singlet-A 6.0405 eV 205.25 nm f=0.0055 <S**2>=0.000
78 -> 88 -0.15282
79 -> 88 0.60996
79 -> 89 -0.22291

Excited State 28: Singlet-A 6.0900 eV 203.59 nm f=0.1421 <S**2>=0.000
72 -> 80 0.64194
76 -> 81 0.22611
77 -> 82 0.11439

Excited State 29: Singlet-A 6.1433 eV 201.82 nm f=0.2030 <S**2>=0.000
70 -> 80 -0.13102
75 -> 81 0.48735
77 -> 83 0.19977
77 -> 84 -0.21609
78 -> 83 -0.13376
78 -> 86 -0.11350
78 -> 88 0.10705
79 -> 91 -0.15966

Excited State 30: Singlet-A 6.1823 eV 200.55 nm f=0.0060 <S**2>=0.000
74 -> 81 0.10743
75 -> 81 0.10868
77 -> 83 -0.20802
77 -> 84 0.21586
78 -> 87 -0.21199
78 -> 89 0.21601
79 -> 85 0.14295
79 -> 89 0.44044
79 -> 90 -0.12231

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0707 eV 403.77 nm f=0.7612 <S**2>=0.000
78 -> 80 -0.12417
79 -> 80 0.69045
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.34254327
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4142 eV 363.14 nm f=0.0853 <S**2>=0.000
78 -> 80 0.68998
79 -> 80 0.12997

Excited State 3: Singlet-A 3.8769 eV 319.80 nm f=0.0097 <S**2>=0.000

73 -> 80 0.61910
74 -> 80 0.20398
75 -> 80 -0.19173

Excited State 4: Singlet-A 4.0920 eV 303.00 nm f=0.3389 <S**2>=0.000
73 -> 80 -0.10366
77 -> 80 0.37991
78 -> 83 0.12184
79 -> 81 0.54753

Excited State 5: Singlet-A 4.1550 eV 298.39 nm f=0.0355 <S**2>=0.000
77 -> 80 0.55852
78 -> 83 -0.14890
79 -> 81 -0.35239
79 -> 83 -0.10920

Excited State 6: Singlet-A 4.2199 eV 293.81 nm f=0.0129 <S**2>=0.000
76 -> 80 0.67207
79 -> 82 -0.15411

Excited State 7: Singlet-A 4.3811 eV 283.00 nm f=0.0500 <S**2>=0.000
78 -> 81 0.63222
79 -> 81 0.15538
79 -> 83 -0.22763

Excited State 8: Singlet-A 4.5341 eV 273.45 nm f=0.0005 <S**2>=0.000
70 -> 80 0.66326
71 -> 80 0.18039

Excited State 9: Singlet-A 4.8046 eV 258.05 nm f=0.0869 <S**2>=0.000
75 -> 80 0.13784
76 -> 80 0.15550
77 -> 81 0.13302
78 -> 81 -0.12362
78 -> 82 -0.16410
78 -> 83 -0.10965
79 -> 82 0.55760
79 -> 83 -0.19786

Excited State 10: Singlet-A 4.8748 eV 254.34 nm f=0.2493 <S**2>=0.000
73 -> 80 0.16023
74 -> 80 -0.16181
75 -> 80 0.41059
77 -> 81 0.14614
78 -> 81 -0.15001
78 -> 83 -0.11421
79 -> 82 -0.29242
79 -> 83 -0.27717

Excited State 11: Singlet-A 4.9346 eV 251.26 nm f=0.2457 <S**2>=0.000
71 -> 80 -0.11754
73 -> 80 0.15378
74 -> 80 -0.18912
75 -> 80 0.37478
77 -> 80 0.13174
77 -> 81 -0.26710
78 -> 81 0.15168
78 -> 83 0.11660
78 -> 84 0.10596

79 -> 82 0.11174
79 -> 83 0.32334

Excited State 12: Singlet-A 5.1819 eV 239.26 nm f=0.0599 <S**2>=0.000
77 -> 81 0.39773
78 -> 83 -0.33391
79 -> 83 0.39331
79 -> 84 -0.18809

Excited State 13: Singlet-A 5.2850 eV 234.60 nm f=0.0445 <S**2>=0.000
74 -> 80 0.41343
75 -> 80 0.22787
77 -> 81 0.10512
78 -> 82 -0.21616
78 -> 83 0.11600
78 -> 86 0.11217
79 -> 84 -0.36419
79 -> 86 0.16978

Excited State 14: Singlet-A 5.3111 eV 233.44 nm f=0.0012 <S**2>=0.000
74 -> 80 0.26605
75 -> 80 0.13948
78 -> 82 0.58461
79 -> 82 0.20207

Excited State 15: Singlet-A 5.3775 eV 230.56 nm f=0.0717 <S**2>=0.000
74 -> 80 0.31710
75 -> 80 0.16171
78 -> 82 -0.20818
78 -> 83 -0.25599
79 -> 83 0.14104
79 -> 84 0.43434
79 -> 85 0.12180

Excited State 16: Singlet-A 5.4160 eV 228.92 nm f=0.0177 <S**2>=0.000
79 -> 85 0.65138
79 -> 88 0.14628

Excited State 17: Singlet-A 5.4925 eV 225.73 nm f=0.0493 <S**2>=0.000
74 -> 80 -0.11608
78 -> 84 -0.20845
78 -> 86 0.18330
79 -> 84 0.10171
79 -> 86 0.58996

Excited State 18: Singlet-A 5.6083 eV 221.07 nm f=0.3093 <S**2>=0.000
75 -> 81 -0.17410
77 -> 81 0.29647
78 -> 83 0.11786
78 -> 84 0.41870
78 -> 86 -0.22659
79 -> 84 0.20506
79 -> 86 0.22016

Excited State 19: Singlet-A 5.6283 eV 220.29 nm f=0.3045 <S**2>=0.000
75 -> 81 0.14471
77 -> 81 -0.24053
78 -> 83 -0.38172
78 -> 84 0.40752

79 -> 83 -0.12305
79 -> 84 -0.14508

Excited State 20: Singlet-A 5.6774 eV 218.38 nm f=0.0121 <S**2>=0.000
78 -> 85 0.48637
78 -> 87 -0.17736
79 -> 87 -0.43882

Excited State 21: Singlet-A 5.7576 eV 215.34 nm f=0.1431 <S**2>=0.000
71 -> 80 -0.30078
74 -> 81 0.12436
77 -> 81 0.11723
78 -> 84 0.16600
78 -> 86 0.51783
79 -> 84 0.13240
79 -> 86 -0.12956

Excited State 22: Singlet-A 5.7957 eV 213.93 nm f=0.0016 <S**2>=0.000
71 -> 80 0.31787
76 -> 81 -0.34564
76 -> 84 -0.13248
77 -> 82 0.41593
78 -> 86 0.11581

Excited State 23: Singlet-A 5.8142 eV 213.24 nm f=0.0857 <S**2>=0.000
70 -> 80 -0.12576
71 -> 80 0.45092
76 -> 81 0.24451
77 -> 82 -0.23440
78 -> 84 0.16115
78 -> 86 0.23826

Excited State 24: Singlet-A 5.8451 eV 212.12 nm f=0.0016 <S**2>=0.000
78 -> 85 0.39092
78 -> 89 0.11463
79 -> 87 0.40269
79 -> 88 0.36999

Excited State 25: Singlet-A 5.8852 eV 210.67 nm f=0.0016 <S**2>=0.000
78 -> 85 -0.19874
78 -> 87 0.15879
78 -> 89 -0.10266
79 -> 85 -0.12055
79 -> 87 -0.30890
79 -> 88 0.53735

Excited State 26: Singlet-A 5.9456 eV 208.53 nm f=0.0010 <S**2>=0.000
72 -> 80 -0.30496
76 -> 81 0.51131
77 -> 82 0.34264

Excited State 27: Singlet-A 6.0153 eV 206.12 nm f=0.0044 <S**2>=0.000
77 -> 85 -0.10030
78 -> 87 0.51431
78 -> 89 0.10854
79 -> 88 -0.13743
79 -> 89 0.38624

Excited State 28: Singlet-A 6.0668 eV 204.36 nm f=0.1160 <S**2>=0.000

72 -> 80 0.61436
76 -> 81 0.20068
77 -> 82 0.22154

Excited State 29: Singlet-A 6.1122 eV 202.85 nm f=0.0407 <S**2>=0.000
75 -> 81 -0.20390
78 -> 87 0.19429
78 -> 88 0.41820
79 -> 85 0.10151
79 -> 89 -0.36865
79 -> 90 -0.20814

Excited State 30: Singlet-A 6.1223 eV 202.51 nm f=0.2308 <S**2>=0.000
75 -> 81 0.52244
77 -> 81 0.10421
77 -> 83 0.14437
77 -> 84 -0.10225
78 -> 83 0.15504
78 -> 87 0.14571
78 -> 88 0.13004
79 -> 84 0.10914
79 -> 89 -0.14918

Single-point TDDFT CAM-B3LYP/6-311++G(2df,2p)/PCM(DMSO) over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometry

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.7267 eV 332.69 nm f=1.0256 <S**2>=0.000
77 -> 80 0.26681
78 -> 80 0.38209
79 -> 80 0.48200
79 -> 81 -0.15748
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.00312977
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9716 eV 312.17 nm f=0.0000 <S**2>=0.000
73 -> 80 0.66237
73 -> 81 0.12931
73 -> 88 -0.12639

Excited State 3: Singlet-A 4.2946 eV 288.70 nm f=0.1531 <S**2>=0.000
77 -> 80 0.13495
78 -> 80 0.35318
78 -> 81 -0.27435
79 -> 80 -0.26415
79 -> 81 0.41826
79 -> 84 -0.10426

Excited State 4: Singlet-A 4.4040 eV 281.53 nm f=0.0494 <S**2>=0.000
77 -> 80 0.16896
77 -> 81 -0.17306
78 -> 81 0.35025
78 -> 84 -0.14340

79 -> 80 0.13089
79 -> 81 0.37846
79 -> 84 0.32515

Excited State 5: Singlet-A 4.5971 eV 269.70 nm f=0.0005 <S**2>=0.000
70 -> 80 0.65875
70 -> 81 0.12731
70 -> 88 -0.12169
74 -> 80 0.10504

Excited State 6: Singlet-A 4.6197 eV 268.38 nm f=0.0027 <S**2>=0.000
76 -> 80 0.60763
77 -> 82 -0.18795
78 -> 82 -0.16157
79 -> 82 -0.14312

Excited State 7: Singlet-A 4.7387 eV 261.64 nm f=0.0322 <S**2>=0.000
76 -> 80 0.11544
77 -> 80 -0.21441
78 -> 80 -0.24947
78 -> 81 -0.23683
79 -> 80 0.39760
79 -> 81 0.30514
79 -> 84 -0.10752
79 -> 88 0.12107

Excited State 8: Singlet-A 5.2122 eV 237.87 nm f=0.6098 <S**2>=0.000
72 -> 80 0.14229
77 -> 80 -0.34853
78 -> 80 0.21015
78 -> 81 -0.19958
78 -> 88 0.13069
79 -> 82 0.16763
79 -> 84 0.41007

Excited State 9: Singlet-A 5.3059 eV 233.67 nm f=0.1926 <S**2>=0.000
76 -> 80 0.18510
77 -> 80 0.33211
77 -> 82 0.17340
78 -> 80 -0.27735
78 -> 81 -0.27825
78 -> 82 0.20396
79 -> 82 0.28259

Excited State 10: Singlet-A 5.4445 eV 227.72 nm f=0.5838 <S**2>=0.000
76 -> 80 0.22435
77 -> 80 -0.17891
77 -> 82 0.21047
78 -> 80 0.16655
78 -> 81 0.24849
78 -> 82 0.30205
79 -> 82 0.25481
79 -> 84 -0.28324

Excited State 11: Singlet-A 5.5679 eV 222.68 nm f=0.0000 <S**2>=0.000
78 -> 85 0.12198
79 -> 83 0.55145
79 -> 85 -0.26692
79 -> 87 -0.20321

79 -> 93 0.12762
79 -> 97 0.12423

Excited State 12: Singlet-A 5.6893 eV 217.92 nm f=0.0281 <S**2>=0.000
78 -> 84 0.10587
78 -> 90 -0.15349
79 -> 88 -0.41426
79 -> 90 0.49840

Excited State 13: Singlet-A 5.8544 eV 211.78 nm f=0.0003 <S**2>=0.000
78 -> 83 0.39607
79 -> 83 0.15073
79 -> 85 0.43701
79 -> 87 -0.18070
79 -> 91 0.10612
79 -> 93 0.10097

Excited State 14: Singlet-A 5.9261 eV 209.22 nm f=0.2715 <S**2>=0.000
77 -> 84 -0.11264
77 -> 88 0.10189
78 -> 82 0.10819
78 -> 84 0.55941
78 -> 88 -0.22660
79 -> 81 0.14677
79 -> 84 0.13972
79 -> 88 0.10537

Excited State 15: Singlet-A 6.0339 eV 205.48 nm f=0.3376 <S**2>=0.000
72 -> 80 -0.10620
76 -> 82 -0.14246
77 -> 81 0.36255
77 -> 90 -0.12327
78 -> 84 -0.12690
78 -> 88 -0.31772
79 -> 82 0.18046
79 -> 84 0.13716
79 -> 88 -0.24849
79 -> 90 -0.12444

Excited State 16: Singlet-A 6.0667 eV 204.37 nm f=0.0007 <S**2>=0.000
78 -> 89 -0.12160
79 -> 86 0.61230
79 -> 89 0.22029

Excited State 17: Singlet-A 6.1270 eV 202.36 nm f=0.0362 <S**2>=0.000
75 -> 80 -0.16177
75 -> 81 0.15831
75 -> 84 -0.18776
77 -> 84 0.15838
77 -> 88 0.13608
77 -> 90 -0.13023
78 -> 84 -0.17508
78 -> 88 -0.18895
78 -> 90 0.37632
79 -> 90 0.22413

Excited State 18: Singlet-A 6.1313 eV 202.21 nm f=0.0015 <S**2>=0.000
77 -> 85 0.11347
78 -> 83 0.38278

78 -> 86 0.12563
78 -> 87 -0.21073
78 -> 93 0.10809
79 -> 85 -0.28947
79 -> 87 0.33181
79 -> 93 -0.10016

Excited State 19: Singlet-A 6.1879 eV 200.37 nm f=0.0004 <S**2>=0.000
66 -> 80 -0.11115
74 -> 80 0.53748
74 -> 81 -0.33763
74 -> 84 0.12949
74 -> 88 0.13082
74 ->100 -0.11299

Excited State 20: Singlet-A 6.1899 eV 200.30 nm f=0.1636 <S**2>=0.000
71 -> 80 0.60341
79 -> 82 0.23966

Excited State 21: Singlet-A 6.2454 eV 198.52 nm f=0.0273 <S**2>=0.000
75 -> 80 -0.29904
75 -> 81 0.47520
76 -> 81 0.10556
77 -> 81 -0.13744
78 -> 90 -0.16960
79 -> 88 -0.14566
79 -> 90 -0.14547

Excited State 22: Singlet-A 6.2700 eV 197.74 nm f=0.0079 <S**2>=0.000
77 -> 83 0.23628
78 -> 83 -0.11594
78 -> 85 0.47071
79 -> 85 0.19142
79 -> 87 0.20387
79 -> 89 -0.13228
79 -> 91 0.12380

Excited State 23: Singlet-A 6.3194 eV 196.20 nm f=0.0415 <S**2>=0.000
71 -> 80 -0.29282
77 -> 82 -0.20820
78 -> 82 -0.28657
78 -> 84 0.10666
79 -> 82 0.42320
79 -> 88 0.10302

Excited State 24: Singlet-A 6.4382 eV 192.58 nm f=0.0003 <S**2>=0.000
78 -> 86 -0.38065
79 -> 83 0.10948
79 -> 86 -0.20152
79 -> 89 0.41865
79 -> 92 0.13346
79 -> 96 0.13357
79 -> 97 -0.10102

Excited State 25: Singlet-A 6.5003 eV 190.73 nm f=0.0129 <S**2>=0.000
75 -> 80 -0.19947
75 -> 81 0.12433
77 -> 81 0.41340
78 -> 81 0.12541

78 -> 88 0.11642
78 -> 90 -0.15017
79 -> 84 0.14089
79 -> 88 0.27033
79 -> 90 0.17225
79 ->100 -0.11024

Excited State 26: Singlet-A 6.5980 eV 187.91 nm f=0.0006 <S**2>=0.000
77 -> 85 0.18642
78 -> 85 -0.32100
78 -> 87 0.34910
78 -> 93 -0.14555
79 -> 83 0.22344
79 -> 87 0.25738
79 -> 89 -0.18859
79 -> 93 -0.10250

Excited State 27: Singlet-A 6.6105 eV 187.56 nm f=0.1374 <S**2>=0.000
72 -> 81 0.10314
75 -> 81 0.13072
76 -> 82 0.51520
77 -> 81 0.13182
77 -> 88 0.10692
79 -> 88 -0.11583
79 -> 90 -0.11768
79 -> 94 -0.22768
79 ->100 0.14449

Excited State 28: Singlet-A 6.7049 eV 184.91 nm f=0.0004 <S**2>=0.000
78 -> 83 -0.12626
78 -> 86 -0.15783
78 -> 87 -0.18834
78 -> 89 0.12484
78 -> 91 -0.14779
79 -> 87 0.16961
79 -> 91 0.41506
79 -> 93 0.32506
79 -> 97 0.11351

Excited State 29: Singlet-A 6.7346 eV 184.10 nm f=0.0117 <S**2>=0.000
65 -> 80 -0.13665
68 -> 80 0.14075
72 -> 80 -0.29821
75 -> 80 0.39218
75 -> 81 0.28561
77 -> 80 -0.18056
77 -> 81 -0.11584
79 -> 88 0.10810
79 -> 90 0.12668
79 ->100 -0.12668

Excited State 30: Singlet-A 6.7529 eV 183.60 nm f=0.0005 <S**2>=0.000
77 -> 83 0.11405
77 -> 85 0.11250
78 -> 83 0.20088
78 -> 86 -0.11546
78 -> 87 0.18271
78 -> 97 -0.13233
79 -> 83 -0.19036

79 -> 91 -0.15295
79 -> 93 0.25450
79 -> 95 -0.11938
79 -> 97 0.36439
79 -> 99 -0.11163
79 ->104 -0.11564

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9348 eV 422.46 nm f=1.3249 <S**2>=0.000
77 -> 80 0.13802
78 -> 80 0.12368
79 -> 80 0.66131
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.56232318
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9244 eV 315.93 nm f=0.0000 <S**2>=0.000
71 -> 80 0.64948
71 -> 81 0.14642
71 -> 92 -0.13246
75 -> 80 -0.13137

Excited State 3: Singlet-A 4.0716 eV 304.51 nm f=0.1782 <S**2>=0.000
77 -> 80 0.17218
77 -> 81 -0.10748
78 -> 80 0.21073
78 -> 81 -0.13409
78 -> 84 -0.11953
78 -> 86 -0.13011
79 -> 81 0.58407

Excited State 4: Singlet-A 4.1711 eV 297.25 nm f=0.0688 <S**2>=0.000
77 -> 81 0.15628
78 -> 80 0.50249
78 -> 81 -0.31244
78 -> 86 0.13265
79 -> 80 -0.12758
79 -> 81 -0.18342
79 -> 84 -0.10627
79 -> 86 -0.15418

Excited State 5: Singlet-A 4.4010 eV 281.72 nm f=0.0063 <S**2>=0.000
76 -> 80 0.50835
77 -> 84 -0.13966
79 -> 84 -0.37832
79 -> 86 0.17601

Excited State 6: Singlet-A 4.5829 eV 270.54 nm f=0.0473 <S**2>=0.000
76 -> 80 0.13517
77 -> 80 0.35238
77 -> 81 -0.11757
78 -> 80 0.23970
78 -> 81 0.30747
79 -> 80 -0.15561
79 -> 81 -0.16725
79 -> 84 0.27084

79 -> 86 0.12247

Excited State 7: Singlet-A 4.6557 eV 266.31 nm f=0.0006 <S**2>=0.000
69 -> 80 0.64693
69 -> 81 0.14452
69 -> 92 -0.12769
75 -> 80 0.14353

Excited State 8: Singlet-A 4.7818 eV 259.28 nm f=0.0956 <S**2>=0.000
76 -> 80 0.41881
77 -> 80 -0.10506
78 -> 80 -0.10250
78 -> 81 -0.26991
78 -> 86 -0.11020
79 -> 84 0.40354

Excited State 9: Singlet-A 4.8106 eV 257.73 nm f=0.0000 <S**2>=0.000
69 -> 80 -0.13892
71 -> 80 0.12475
75 -> 80 0.62985
75 -> 92 0.18110

Excited State 10: Singlet-A 4.8540 eV 255.43 nm f=0.0009 <S**2>=0.000
79 -> 82 0.55703
79 -> 83 0.24972
79 -> 87 -0.20210
79 -> 93 -0.15356

Excited State 11: Singlet-A 4.9187 eV 252.07 nm f=0.4856 <S**2>=0.000
72 -> 80 0.12285
76 -> 80 -0.12794
77 -> 80 -0.22693
77 -> 81 -0.11382
78 -> 80 0.14079
78 -> 81 -0.14076
78 -> 84 -0.16044
78 -> 86 -0.13497
79 -> 81 -0.10198
79 -> 86 0.48508
79 -> 89 0.11312
79 -> 92 0.13730

Excited State 12: Singlet-A 5.0008 eV 247.93 nm f=0.0947 <S**2>=0.000
77 -> 80 0.43415
78 -> 80 -0.27995
78 -> 81 -0.32991
78 -> 84 -0.10279
79 -> 81 -0.15717
79 -> 84 -0.10352
79 -> 89 0.13701

Excited State 13: Singlet-A 5.2386 eV 236.68 nm f=0.0037 <S**2>=0.000
77 -> 82 0.11333
78 -> 82 0.29238
79 -> 82 -0.14410
79 -> 83 0.48962
79 -> 85 -0.18288
79 -> 87 0.18972
79 -> 90 0.13143

Excited State 14: Singlet-A 5.3594 eV 231.34 nm f=0.0590 <S**2>=0.000
77 -> 81 -0.10680
77 -> 89 -0.13449
78 -> 81 0.15282
78 -> 89 -0.18770
78 -> 92 0.12787
79 -> 86 -0.16587
79 -> 89 0.53058
79 -> 92 -0.16247

Excited State 15: Singlet-A 5.4186 eV 228.81 nm f=0.0036 <S**2>=0.000
79 -> 83 0.20193
79 -> 85 0.56707
79 -> 88 0.24933

Excited State 16: Singlet-A 5.5003 eV 225.41 nm f=0.1271 <S**2>=0.000
77 -> 81 -0.21512
77 -> 86 0.10986
78 -> 84 -0.15426
78 -> 86 -0.30724
78 -> 89 0.31641
79 -> 81 -0.14421
79 -> 84 -0.18186
79 -> 86 -0.29698
79 -> 89 -0.13626
79 -> 92 0.11628

Excited State 17: Singlet-A 5.5260 eV 224.37 nm f=0.0011 <S**2>=0.000
78 -> 82 -0.31414
78 -> 83 0.27635
79 -> 82 0.15805
79 -> 85 -0.12357
79 -> 87 0.43066
79 -> 93 0.13683

Excited State 18: Singlet-A 5.6342 eV 220.06 nm f=0.3532 <S**2>=0.000
77 -> 81 -0.10551
78 -> 81 0.10022
78 -> 84 0.20215
78 -> 86 0.22386
78 -> 89 0.12488
79 -> 89 0.22300
79 -> 92 0.50257

Excited State 19: Singlet-A 5.6560 eV 219.21 nm f=0.0003 <S**2>=0.000
73 -> 80 0.61490
73 -> 81 -0.23000
73 -> 89 0.10337
73 -> 92 0.11249

Excited State 20: Singlet-A 5.6721 eV 218.59 nm f=0.0020 <S**2>=0.000
77 -> 82 -0.11886
77 -> 83 0.13170
78 -> 82 0.37381
78 -> 85 -0.10170
78 -> 87 -0.21168
78 -> 93 -0.10146
79 -> 82 0.27681

79 -> 83 -0.23546
79 -> 87 0.22563
79 -> 88 0.10841
79 -> 93 0.10457

Excited State 21: Singlet-A 5.7478 eV 215.71 nm f=0.0000 <S**2>=0.000
78 -> 85 0.30109
79 -> 85 -0.16542
79 -> 87 -0.17888
79 -> 88 0.53363
79 -> 91 -0.11148

Excited State 22: Singlet-A 5.8143 eV 213.24 nm f=0.0389 <S**2>=0.000
77 -> 89 -0.19143
78 -> 84 0.14268
78 -> 86 0.10552
78 -> 89 0.46624
78 -> 92 -0.19769
79 -> 89 0.15512
79 -> 92 -0.24986

Excited State 23: Singlet-A 5.9531 eV 208.27 nm f=0.0003 <S**2>=0.000
78 -> 83 -0.31619
78 -> 87 0.35044
78 -> 93 0.11672
79 -> 90 -0.30714
79 -> 93 0.13182
79 -> 94 0.16748

Excited State 24: Singlet-A 5.9789 eV 207.37 nm f=0.4712 <S**2>=0.000
70 -> 80 0.14571
72 -> 80 -0.14501
74 -> 80 0.26203
74 -> 81 -0.17421
77 -> 81 0.40822
78 -> 84 -0.20176
78 -> 86 -0.17130
78 -> 89 0.12680
79 -> 92 0.14830
79 -> 95 -0.11802

Excited State 25: Singlet-A 6.0234 eV 205.84 nm f=0.0428 <S**2>=0.000
74 -> 80 0.13705
79 -> 95 0.63284

Excited State 26: Singlet-A 6.0473 eV 205.03 nm f=0.2314 <S**2>=0.000
70 -> 80 0.63686
70 -> 81 0.10886
79 -> 95 0.11180

Excited State 27: Singlet-A 6.0488 eV 204.97 nm f=0.0001 <S**2>=0.000
78 -> 85 -0.22961
78 -> 87 -0.12618
79 -> 85 -0.15231
79 -> 87 -0.23166
79 -> 93 0.41814
79 -> 94 0.28400

Excited State 28: Singlet-A 6.0751 eV 204.09 nm f=0.0011 <S**2>=0.000

78 -> 85 0.40661
78 -> 88 -0.21607
79 -> 88 -0.12485
79 -> 90 0.21158
79 -> 91 0.26572
79 -> 93 0.23733
79 -> 94 0.11750

Excited State 29: Singlet-A 6.1901 eV 200.30 nm f=0.0000 <S**2>=0.000
77 -> 87 -0.14290
78 -> 83 -0.30828
78 -> 85 -0.18220
78 -> 87 0.13726
78 -> 88 0.14151
78 -> 93 0.12491
79 -> 83 -0.13504
79 -> 88 0.12363
79 -> 90 0.39420
79 -> 96 0.12402

Excited State 30: Singlet-A 6.1958 eV 200.11 nm f=0.0757 <S**2>=0.000
74 -> 80 0.42159
74 -> 81 -0.27743
77 -> 80 -0.10934
77 -> 81 -0.32782
79 -> 95 -0.10990

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.6562 eV 339.10 nm f=1.1559 <S**2>=0.000
77 -> 80 0.24057
78 -> 80 0.31744
79 -> 80 0.53887
79 -> 81 -0.16411
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.00296517
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9694 eV 312.35 nm f=0.0000 <S**2>=0.000
73 -> 80 0.66520
73 -> 81 0.13594
73 -> 88 -0.12102

Excited State 3: Singlet-A 4.2913 eV 288.92 nm f=0.0154 <S**2>=0.000
77 -> 80 0.15347
78 -> 80 0.37381
78 -> 81 -0.26212
79 -> 80 -0.17860
79 -> 81 0.45207

Excited State 4: Singlet-A 4.3518 eV 284.91 nm f=0.0344 <S**2>=0.000
77 -> 80 0.12432
77 -> 81 -0.17112
78 -> 80 -0.14983
78 -> 81 0.32175
78 -> 84 -0.14704
79 -> 80 0.18364

79 -> 81 0.38490
79 -> 84 0.31229

Excited State 5: Singlet-A 4.5985 eV 269.62 nm f=0.0005 <S**2>=0.000
70 -> 80 0.66626
70 -> 81 0.13433
70 -> 88 -0.11674

Excited State 6: Singlet-A 4.6277 eV 267.92 nm f=0.0057 <S**2>=0.000
76 -> 80 0.60580
77 -> 82 -0.19064
78 -> 82 -0.17782
79 -> 82 -0.19227

Excited State 7: Singlet-A 4.7685 eV 260.01 nm f=0.0693 <S**2>=0.000
77 -> 80 -0.24085
78 -> 80 -0.29566
78 -> 81 -0.29199
79 -> 80 0.35455
79 -> 81 0.24620
79 -> 84 -0.15354
79 -> 88 0.13527

Excited State 8: Singlet-A 5.1783 eV 239.43 nm f=0.5896 <S**2>=0.000
72 -> 80 0.14748
77 -> 80 -0.34804
77 -> 81 -0.10259
78 -> 80 0.19507
78 -> 81 -0.21027
78 -> 88 0.12587
79 -> 84 0.44427

Excited State 9: Singlet-A 5.2655 eV 235.46 nm f=0.0803 <S**2>=0.000
76 -> 80 0.22769
77 -> 80 0.31055
77 -> 82 0.17142
78 -> 80 -0.22842
78 -> 81 -0.23837
78 -> 82 0.21244
79 -> 82 0.32386
79 -> 84 0.11407

Excited State 10: Singlet-A 5.3816 eV 230.39 nm f=0.5889 <S**2>=0.000
76 -> 80 0.22652
77 -> 80 -0.23384
77 -> 82 0.16979
78 -> 80 0.19950
78 -> 81 0.28233
78 -> 82 0.21739
79 -> 82 0.32486
79 -> 84 -0.20987

Excited State 11: Singlet-A 5.4831 eV 226.12 nm f=0.0001 <S**2>=0.000
78 -> 85 -0.11342
79 -> 83 0.56625
79 -> 85 0.16998
79 -> 86 -0.14035
79 -> 87 -0.22524
79 -> 93 -0.12861

79 -> 97 0.10838

Excited State 12: Singlet-A 5.6527 eV 219.34 nm f=0.0299 <S**2>=0.000
78 -> 84 0.10402
78 -> 90 -0.15927
79 -> 88 -0.40605
79 -> 90 0.49726

Excited State 13: Singlet-A 5.7666 eV 215.00 nm f=0.0009 <S**2>=0.000
77 -> 83 -0.10100
78 -> 83 -0.32089
78 -> 85 -0.10047
79 -> 85 0.51797
79 -> 86 0.10076
79 -> 87 0.11218
79 -> 91 -0.14503

Excited State 14: Singlet-A 5.9196 eV 209.45 nm f=0.2527 <S**2>=0.000
75 -> 84 -0.10816
77 -> 88 0.12514
78 -> 84 0.52946
78 -> 88 -0.25633
78 -> 90 0.11722
79 -> 81 0.12584
79 -> 84 0.16107
79 -> 88 0.13772

Excited State 15: Singlet-A 6.0366 eV 205.39 nm f=0.3989 <S**2>=0.000
72 -> 80 -0.10470
76 -> 82 -0.12108
77 -> 81 0.38733
78 -> 84 -0.11740
78 -> 88 -0.26798
79 -> 84 0.16756
79 -> 88 -0.29470
79 -> 90 -0.21121

Excited State 16: Singlet-A 6.0381 eV 205.34 nm f=0.0002 <S**2>=0.000
78 -> 86 -0.10916
78 -> 89 0.10872
79 -> 83 0.14006
79 -> 86 0.58566
79 -> 89 -0.25565

Excited State 17: Singlet-A 6.1323 eV 202.18 nm f=0.0469 <S**2>=0.000
75 -> 80 -0.16846
75 -> 81 0.16053
75 -> 84 -0.16822
77 -> 84 0.16019
77 -> 90 -0.15645
78 -> 82 -0.11427
78 -> 84 -0.27114
78 -> 88 -0.21614
78 -> 90 0.31785
79 -> 82 0.11725
79 -> 90 0.20371

Excited State 18: Singlet-A 6.1445 eV 201.78 nm f=0.0004 <S**2>=0.000
77 -> 85 -0.12341

78 -> 83 0.37653
78 -> 87 -0.19960
78 -> 93 -0.10595
79 -> 85 0.22761
79 -> 87 0.36675
79 -> 91 0.10359
79 -> 93 0.11822

Excited State 19: Singlet-A 6.1754 eV 200.77 nm f=0.0641 <S**2>=0.000
71 -> 80 0.51552
75 -> 80 0.13771
75 -> 81 -0.19114
77 -> 81 0.14957
78 -> 88 0.11273
79 -> 82 0.23747

Excited State 20: Singlet-A 6.1985 eV 200.02 nm f=0.1443 <S**2>=0.000
71 -> 80 0.33658
75 -> 80 -0.21906
75 -> 81 0.35199
77 -> 81 -0.18961
77 -> 84 -0.12346
78 -> 88 -0.11106
78 -> 90 -0.14255
79 -> 88 -0.18243
79 -> 90 -0.17440

Excited State 21: Singlet-A 6.2290 eV 199.04 nm f=0.0046 <S**2>=0.000
77 -> 83 -0.18531
78 -> 83 0.25933
78 -> 85 0.40253
78 -> 87 -0.12003
79 -> 85 0.18687
79 -> 86 0.10310
79 -> 87 -0.23315
79 -> 91 -0.13638

Excited State 22: Singlet-A 6.3152 eV 196.33 nm f=0.0644 <S**2>=0.000
71 -> 80 -0.26816
75 -> 81 0.13380
77 -> 82 -0.18027
78 -> 82 -0.34952
78 -> 90 -0.20685
79 -> 82 0.36984

Excited State 23: Singlet-A 6.3764 eV 194.44 nm f=0.0000 <S**2>=0.000
74 -> 80 0.45137
74 -> 81 -0.43587
74 -> 84 0.13654
74 -> 88 0.10215
74 -> 95 0.10137
74 ->100 -0.14153
79 -> 89 0.11914

Excited State 24: Singlet-A 6.3981 eV 193.78 nm f=0.0093 <S**2>=0.000
74 -> 80 -0.11374
74 -> 81 0.11407
77 -> 83 0.12429
78 -> 85 -0.12461

78 -> 86 0.28699
79 -> 83 0.12419
79 -> 85 -0.11004
79 -> 86 0.19173
79 -> 89 0.45426
79 -> 92 -0.11895
79 -> 96 0.12817

Excited State 25: Singlet-A 6.4945 eV 190.91 nm f=0.0684 <S**2>=0.000
75 -> 80 -0.25461
75 -> 81 0.19241
76 -> 82 -0.13786
77 -> 81 0.31663
77 -> 88 -0.10001
78 -> 81 0.11184
78 -> 82 0.20338
78 -> 90 -0.16436
79 -> 82 -0.12869
79 -> 88 0.25898
79 -> 90 0.14027
79 ->100 -0.13148

Excited State 26: Singlet-A 6.5692 eV 188.74 nm f=0.0029 <S**2>=0.000
77 -> 85 -0.17700
78 -> 85 0.31985
78 -> 87 0.33638
78 -> 93 0.11109
79 -> 83 0.22919
79 -> 87 0.18956
79 -> 91 -0.12165
79 -> 93 0.23051
79 -> 97 -0.13697

Excited State 27: Singlet-A 6.5708 eV 188.69 nm f=0.1472 <S**2>=0.000
72 -> 81 0.11895
75 -> 80 -0.13086
75 -> 81 0.11491
76 -> 82 0.44714
77 -> 81 0.20473
78 -> 88 0.11483
79 -> 95 -0.30240
79 ->100 0.15388

Excited State 28: Singlet-A 6.6461 eV 186.55 nm f=0.0001 <S**2>=0.000
78 -> 85 -0.18915
78 -> 86 -0.23768
78 -> 91 0.11336
79 -> 87 -0.24166
79 -> 91 -0.30100
79 -> 93 0.30269
79 -> 97 -0.25018

Excited State 29: Singlet-A 6.7116 eV 184.73 nm f=0.0899 <S**2>=0.000
65 -> 80 0.13783
68 -> 80 0.14449
72 -> 80 -0.30709
75 -> 80 0.33765
75 -> 81 0.27866
76 -> 82 0.18656

77 -> 80 -0.20241
79 -> 90 0.10742
79 -> 95 0.10317
79 ->100 -0.10159

Excited State 30: Singlet-A 6.7382 eV 184.00 nm f=0.0018 <S**2>=0.000
77 -> 83 -0.10685
78 -> 83 -0.20246
78 -> 85 0.12599
78 -> 87 -0.17597
78 -> 97 0.11545
79 -> 83 0.14372
79 -> 91 0.33153
79 -> 93 0.15060
79 -> 97 -0.30835
79 -> 99 -0.14353

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9069 eV 426.52 nm f=1.3798 <S**2>=0.000
77 -> 80 0.12578
78 -> 80 -0.14365
79 -> 80 0.65738
79 -> 81 0.10206
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.55981255
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9246 eV 315.92 nm f=0.0023 <S**2>=0.000
71 -> 80 -0.18322
72 -> 80 0.62235
72 -> 81 -0.13902
72 -> 92 -0.11802
75 -> 80 -0.11656

Excited State 3: Singlet-A 4.0246 eV 308.06 nm f=0.1112 <S**2>=0.000
77 -> 80 -0.17317
77 -> 81 -0.11965
78 -> 80 0.11064
78 -> 86 -0.17246
79 -> 81 0.61555

Excited State 4: Singlet-A 4.1601 eV 298.03 nm f=0.0069 <S**2>=0.000
77 -> 81 0.12989
78 -> 80 0.53243
78 -> 81 0.30254
78 -> 86 0.10633
79 -> 80 0.14198
79 -> 86 0.18883

Excited State 5: Singlet-A 4.3900 eV 282.42 nm f=0.0013 <S**2>=0.000
75 -> 80 0.10550
76 -> 80 -0.43085
77 -> 84 0.15670
78 -> 84 -0.13494
79 -> 84 0.45929

Excited State 6: Singlet-A 4.4560 eV 278.24 nm f=0.0696 <S**2>=0.000
75 -> 80 -0.26499
77 -> 80 0.49770
78 -> 81 0.23483
79 -> 80 -0.12776
79 -> 81 0.16546
79 -> 86 0.13146

Excited State 7: Singlet-A 4.6693 eV 265.53 nm f=0.0030 <S**2>=0.000
69 -> 80 0.65168
69 -> 81 -0.14428
69 -> 92 -0.11990

Excited State 8: Singlet-A 4.6985 eV 263.88 nm f=0.0547 <S**2>=0.000
76 -> 80 0.37987
78 -> 80 -0.12828
79 -> 82 0.31900
79 -> 83 0.13670
79 -> 84 0.23513
79 -> 86 0.24409

Excited State 9: Singlet-A 4.7704 eV 259.91 nm f=0.0983 <S**2>=0.000
75 -> 80 0.22771
76 -> 80 -0.18845
77 -> 80 -0.15873
78 -> 80 -0.31083
78 -> 81 0.20354
79 -> 82 -0.13228
79 -> 84 -0.18069
79 -> 86 0.34030

Excited State 10: Singlet-A 4.8107 eV 257.73 nm f=0.0090 <S**2>=0.000
76 -> 80 -0.27191
79 -> 82 0.43273
79 -> 83 0.11081
79 -> 84 -0.28609
79 -> 85 -0.13037
79 -> 87 0.19242
79 -> 88 0.12886
79 -> 93 -0.10733

Excited State 11: Singlet-A 4.9086 eV 252.59 nm f=0.4633 <S**2>=0.000
74 -> 80 -0.10411
76 -> 80 0.14191
78 -> 80 -0.17998
78 -> 81 0.45034
78 -> 86 -0.13350
79 -> 81 -0.10714
79 -> 84 0.10271
79 -> 86 -0.28103
79 -> 89 -0.17457
79 -> 92 -0.13336

Excited State 12: Singlet-A 5.1608 eV 240.24 nm f=0.0111 <S**2>=0.000
71 -> 80 -0.19339
74 -> 80 -0.20345
75 -> 80 0.40487
77 -> 80 0.27586
78 -> 86 0.10601

79 -> 81 0.10305
79 -> 83 -0.17617
79 -> 89 0.12037

Excited State 13: Singlet-A 5.1748 eV 239.59 nm f=0.0084 <S**2>=0.000
75 -> 80 0.14033
77 -> 82 0.10603
78 -> 82 -0.23701
79 -> 83 0.50685
79 -> 87 -0.19351
79 -> 90 -0.10268
79 -> 97 0.10435

Excited State 14: Singlet-A 5.2917 eV 234.30 nm f=0.0299 <S**2>=0.000
77 -> 89 -0.11330
78 -> 81 0.13158
78 -> 89 0.15947
79 -> 85 0.16106
79 -> 88 -0.19903
79 -> 89 0.47057
79 -> 90 0.11781
79 -> 92 -0.18060

Excited State 15: Singlet-A 5.3787 eV 230.51 nm f=0.0228 <S**2>=0.000
79 -> 82 0.22928
79 -> 84 -0.10726
79 -> 85 0.51354
79 -> 86 0.12002
79 -> 88 -0.17107
79 -> 89 -0.20500

Excited State 16: Singlet-A 5.4912 eV 225.79 nm f=0.0160 <S**2>=0.000
77 -> 81 -0.15280
78 -> 82 -0.17929
78 -> 83 0.20177
78 -> 86 -0.16669
78 -> 89 0.11974
79 -> 82 -0.15329
79 -> 85 0.16937
79 -> 86 0.20272
79 -> 87 0.38064
79 -> 88 0.10369
79 -> 93 -0.14058

Excited State 17: Singlet-A 5.5036 eV 225.28 nm f=0.1055 <S**2>=0.000
77 -> 81 0.22008
77 -> 86 0.10365
78 -> 83 0.13387
78 -> 86 0.33863
78 -> 89 -0.23280
79 -> 81 0.13227
79 -> 85 0.12965
79 -> 86 -0.21483
79 -> 87 0.20468
79 -> 88 0.10635
79 -> 89 -0.11336

Excited State 18: Singlet-A 5.5926 eV 221.69 nm f=0.3645 <S**2>=0.000
77 -> 81 0.16043

78 -> 81 0.13100
78 -> 86 -0.19051
78 -> 89 -0.12433
79 -> 85 0.11683
79 -> 89 0.22271
79 -> 90 -0.13117
79 -> 91 -0.12110
79 -> 92 0.47283

Excited State 19: Singlet-A 5.6466 eV 219.57 nm f=0.0054 <S**2>=0.000
78 -> 82 0.18801
78 -> 85 0.21429
79 -> 85 0.17286
79 -> 87 -0.21909
79 -> 88 0.45810
79 -> 90 -0.10549
79 -> 91 0.16785
79 -> 94 0.12107

Excited State 20: Singlet-A 5.6893 eV 217.93 nm f=0.0047 <S**2>=0.000
77 -> 82 0.14138
78 -> 82 0.44410
78 -> 87 0.17968
78 -> 88 0.15025
78 -> 97 -0.10297
79 -> 82 -0.13845
79 -> 83 0.26985
79 -> 87 0.18937

Excited State 21: Singlet-A 5.8469 eV 212.05 nm f=0.0498 <S**2>=0.000
77 -> 86 0.10177
77 -> 89 0.14366
78 -> 84 0.11674
78 -> 86 0.15569
78 -> 88 -0.10176
78 -> 89 0.42230
78 -> 92 -0.16696
79 -> 89 -0.14985
79 -> 92 0.22213
79 -> 94 0.15439

Excited State 22: Singlet-A 5.8766 eV 210.98 nm f=0.0678 <S**2>=0.000
73 -> 80 0.53909
73 -> 81 0.30054
73 -> 86 0.10690
77 -> 81 0.16762

Excited State 23: Singlet-A 5.8937 eV 210.37 nm f=0.0948 <S**2>=0.000
77 -> 81 0.17179
78 -> 86 -0.20360
78 -> 87 0.12624
79 -> 83 0.10969
79 -> 90 0.23574
79 -> 93 0.23628
79 -> 94 0.39700

Excited State 24: Singlet-A 5.9149 eV 209.61 nm f=0.4431 <S**2>=0.000
73 -> 80 -0.18528
73 -> 81 -0.10007

74 -> 80 0.10499
74 -> 81 0.11397
75 -> 80 0.10743
77 -> 81 0.38850
77 -> 89 0.11181
78 -> 81 -0.11012
78 -> 86 -0.21405
78 -> 89 0.15971
79 -> 92 -0.17730
79 -> 94 -0.13363

Excited State 25: Singlet-A 5.9609 eV 208.00 nm f=0.0085 <S**2>=0.000
78 -> 83 0.31783
78 -> 85 0.15792
78 -> 87 0.20241
78 -> 88 0.13952
79 -> 88 0.10755
79 -> 90 0.27771
79 -> 91 -0.15756
79 -> 94 -0.21945
79 -> 95 0.15818
79 -> 96 -0.11855

Excited State 26: Singlet-A 6.0211 eV 205.92 nm f=0.1945 <S**2>=0.000
70 -> 80 0.59807
70 -> 81 -0.10234
77 -> 84 0.15133
79 -> 84 -0.10490
79 -> 93 0.10863

Excited State 27: Singlet-A 6.0406 eV 205.25 nm f=0.0082 <S**2>=0.000
70 -> 80 -0.15087
79 -> 87 0.11571
79 -> 90 -0.10748
79 -> 93 0.44434
79 -> 94 -0.16205
79 -> 95 0.29657
79 -> 96 -0.11958

Excited State 28: Singlet-A 6.1076 eV 203.00 nm f=0.0030 <S**2>=0.000
78 -> 83 -0.11583
78 -> 85 -0.30875
78 -> 88 -0.16405
79 -> 88 0.12127
79 -> 90 0.16007
79 -> 91 0.31858
79 -> 94 -0.21251
79 -> 95 0.15040
79 -> 96 0.11519
79 -> 97 -0.11542

Excited State 29: Singlet-A 6.1440 eV 201.80 nm f=0.0112 <S**2>=0.000
70 -> 80 0.15806
71 -> 80 0.14873
74 -> 80 0.35560
74 -> 81 0.19602
75 -> 80 0.16653
75 -> 81 0.24687
75 -> 84 0.12029

76 -> 81 0.10606
77 -> 81 -0.10874
77 -> 84 -0.15801
78 -> 84 0.10506
79 -> 90 -0.11796

Excited State 30: Singlet-A 6.1683 eV 201.00 nm f=0.0029 <S**2>=0.000
74 -> 80 0.11319
78 -> 83 -0.29776
78 -> 87 -0.16920
78 -> 93 0.12897
79 -> 88 0.19720
79 -> 90 0.30901
79 -> 91 -0.26522

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.6913 eV 335.88 nm f=0.9529 <S**2>=0.000
77 -> 80 0.28733
78 -> 80 0.31503
79 -> 80 0.51862
79 -> 81 0.12811
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1043.99745455
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9637 eV 312.80 nm f=0.0110 <S**2>=0.000
73 -> 80 0.65472
73 -> 87 0.13012

Excited State 3: Singlet-A 4.3885 eV 282.52 nm f=0.1118 <S**2>=0.000
77 -> 80 -0.22550
77 -> 81 -0.15972
78 -> 80 -0.11744
78 -> 84 -0.24753
79 -> 81 0.53623
79 -> 84 0.16456

Excited State 4: Singlet-A 4.4724 eV 277.22 nm f=0.0756 <S**2>=0.000
77 -> 81 -0.10924
78 -> 80 0.30931
78 -> 81 0.48997
79 -> 80 -0.24601
79 -> 81 -0.11139
79 -> 84 0.22657

Excited State 5: Singlet-A 4.5621 eV 271.77 nm f=0.0158 <S**2>=0.000
76 -> 80 0.61631
77 -> 82 -0.18926
78 -> 82 -0.11967
79 -> 82 -0.16104

Excited State 6: Singlet-A 4.5986 eV 269.61 nm f=0.0003 <S**2>=0.000
70 -> 80 0.65922
70 -> 87 0.12659
71 -> 80 -0.10068

Excited State 7: Singlet-A 4.7126 eV 263.09 nm f=0.0180 <S**2>=0.000
75 -> 80 -0.17218
76 -> 80 0.11077
77 -> 80 0.42303
78 -> 80 0.10646
78 -> 81 -0.19497
79 -> 80 -0.33409
79 -> 81 0.24453

Excited State 8: Singlet-A 4.9366 eV 251.15 nm f=0.0245 <S**2>=0.000
74 -> 80 0.12639
77 -> 80 -0.30422
78 -> 80 0.49609
78 -> 81 -0.23055
79 -> 80 -0.14122
79 -> 84 -0.13961

Excited State 9: Singlet-A 5.2916 eV 234.30 nm f=0.5676 <S**2>=0.000
76 -> 80 -0.18434
77 -> 81 -0.11100
77 -> 82 -0.17925
78 -> 81 -0.22456
78 -> 82 -0.20591
78 -> 84 -0.17196
79 -> 81 -0.16888
79 -> 82 -0.28601
79 -> 84 0.30899
79 -> 87 0.10906

Excited State 10: Singlet-A 5.3231 eV 232.92 nm f=0.7011 <S**2>=0.000
76 -> 80 0.22270
77 -> 82 0.20939
78 -> 81 -0.21059
78 -> 82 0.20531
78 -> 84 -0.17113
79 -> 81 -0.14199
79 -> 82 0.37652
79 -> 84 0.26094

Excited State 11: Singlet-A 5.6167 eV 220.74 nm f=0.0056 <S**2>=0.000
78 -> 85 0.12181
79 -> 83 0.59259
79 -> 88 -0.17294
79 -> 89 -0.14079

Excited State 12: Singlet-A 5.7323 eV 216.29 nm f=0.0901 <S**2>=0.000
77 -> 84 -0.12455
78 -> 84 0.36116
78 -> 90 -0.13953
79 -> 81 0.11559
79 -> 84 0.30766
79 -> 88 -0.10484
79 -> 89 0.21291
79 -> 90 0.30721

Excited State 13: Singlet-A 5.7897 eV 214.15 nm f=0.2322 <S**2>=0.000
71 -> 80 -0.16508
77 -> 81 0.26179
77 -> 84 -0.11745

77 -> 86 0.12651
77 -> 87 -0.17663
78 -> 83 0.13085
78 -> 86 0.12751
78 -> 87 -0.15267
79 -> 84 0.24636
79 -> 86 0.21050
79 -> 87 -0.18772
79 -> 89 -0.11346
79 -> 90 -0.19538

Excited State 14: Singlet-A 5.8262 eV 212.80 nm f=0.2113 <S**2>=0.000
78 -> 84 0.34505
78 -> 88 -0.10714
78 -> 89 0.16264
78 -> 90 0.28931
79 -> 81 0.11802
79 -> 84 0.15203
79 -> 87 0.18354
79 -> 88 0.11007
79 -> 89 -0.16016
79 -> 90 -0.23579

Excited State 15: Singlet-A 5.8438 eV 212.16 nm f=0.0173 <S**2>=0.000
78 -> 83 0.45734
78 -> 85 -0.22543
78 -> 89 -0.10203
79 -> 85 0.31944
79 -> 92 0.11262

Excited State 16: Singlet-A 5.9818 eV 207.27 nm f=0.0008 <S**2>=0.000
71 -> 80 0.24023
74 -> 80 0.28046
75 -> 80 0.35798
75 -> 87 -0.10266
77 -> 80 0.18550
78 -> 80 -0.11516
79 -> 80 -0.14343
79 -> 86 0.15589
79 -> 87 -0.13225

Excited State 17: Singlet-A 6.0597 eV 204.60 nm f=0.3015 <S**2>=0.000
74 -> 84 -0.12359
75 -> 84 0.13986
77 -> 81 0.14440
77 -> 90 -0.14513
78 -> 84 -0.22685
78 -> 87 -0.11088
78 -> 88 -0.12839
78 -> 89 0.22301
78 -> 90 0.34211
79 -> 89 0.14924
79 -> 90 0.20564

Excited State 18: Singlet-A 6.1320 eV 202.19 nm f=0.0042 <S**2>=0.000
72 -> 80 0.33804
75 -> 82 0.11483
77 -> 81 -0.12239
77 -> 82 -0.24591

78 -> 83 0.14396
78 -> 88 -0.10646
79 -> 82 0.22016
79 -> 85 -0.25188
79 -> 86 0.20612

Excited State 19: Singlet-A 6.1691 eV 200.98 nm f=0.0467 <S**2>=0.000
72 -> 80 0.36243
77 -> 82 -0.12217
78 -> 83 -0.19983
78 -> 88 0.15424
78 -> 89 0.12956
79 -> 82 0.16255
79 -> 85 0.35209
79 -> 86 -0.15801

Excited State 20: Singlet-A 6.2013 eV 199.93 nm f=0.0776 <S**2>=0.000
72 -> 80 0.16885
75 -> 80 0.10119
77 -> 81 0.34496
77 -> 83 -0.14822
78 -> 85 -0.20511
78 -> 87 0.15906
79 -> 85 -0.20177
79 -> 86 -0.30835

Excited State 21: Singlet-A 6.2522 eV 198.31 nm f=0.0221 <S**2>=0.000
72 -> 80 -0.13000
77 -> 81 0.20449
78 -> 85 -0.12884
78 -> 86 -0.27065
78 -> 87 -0.11896
78 -> 88 0.17542
79 -> 86 0.24203
79 -> 87 0.34327
79 -> 88 -0.17521

Excited State 22: Singlet-A 6.2568 eV 198.16 nm f=0.0811 <S**2>=0.000
72 -> 80 0.26526
77 -> 81 0.18252
77 -> 82 0.18047
77 -> 83 0.16374
78 -> 85 0.33898
78 -> 86 -0.13604
79 -> 87 0.15797
79 -> 88 0.17515
79 -> 89 0.16314

Excited State 23: Singlet-A 6.2957 eV 196.94 nm f=0.0492 <S**2>=0.000
72 -> 80 0.31113
74 -> 82 -0.10265
75 -> 82 -0.15750
77 -> 81 -0.12554
77 -> 82 0.30135
77 -> 83 -0.16702
78 -> 85 -0.19814
78 -> 87 -0.12567
79 -> 82 -0.22909
79 -> 86 0.15472

79 -> 88 -0.14671

Excited State 24: Singlet-A 6.4512 eV 192.19 nm f=0.0193 <S**2>=0.000
74 -> 80 -0.19376
74 -> 81 -0.30144
75 -> 80 0.12288
75 -> 81 0.35741
78 -> 86 0.19223
78 -> 87 0.19586
79 -> 86 0.12438
79 -> 91 -0.19385

Excited State 25: Singlet-A 6.4602 eV 191.92 nm f=0.0052 <S**2>=0.000
74 -> 80 0.14883
74 -> 81 0.24648
75 -> 80 -0.12011
75 -> 81 -0.24427
77 -> 85 -0.12164
78 -> 83 -0.11562
78 -> 85 0.11231
78 -> 86 0.25748
78 -> 87 0.13850
78 -> 88 -0.11773
79 -> 86 0.11214
79 -> 87 0.16031
79 -> 89 -0.12484
79 -> 90 0.13400
79 -> 91 -0.15849
79 -> 96 -0.10101

Excited State 26: Singlet-A 6.4930 eV 190.95 nm f=0.0352 <S**2>=0.000
76 -> 82 0.32829
77 -> 87 -0.13278
78 -> 89 0.13091
79 -> 86 -0.11164
79 -> 88 -0.10117
79 -> 89 0.22630
79 -> 91 -0.25437
79 -> 93 -0.20526

Excited State 27: Singlet-A 6.5391 eV 189.61 nm f=0.0027 <S**2>=0.000
77 -> 83 0.12028
77 -> 85 0.20938
78 -> 85 -0.20156
78 -> 86 0.22749
78 -> 87 0.10924
78 -> 88 0.26008
78 -> 89 0.13949
79 -> 83 0.12781
79 -> 86 0.14271
79 -> 88 0.30020
79 -> 90 0.10432

Excited State 28: Singlet-A 6.5939 eV 188.03 nm f=0.0043 <S**2>=0.000
74 -> 82 0.13125
77 -> 82 -0.18016
78 -> 82 0.49643
78 -> 83 -0.11819
78 -> 87 -0.14236

79 -> 82 -0.19710
79 -> 87 0.13944
79 -> 91 0.10790

Excited State 29: Singlet-A 6.6365 eV 186.82 nm f=0.1673 <S**2>=0.000
76 -> 82 0.43686
76 -> 83 -0.10328
77 -> 86 0.10634
78 -> 82 -0.13456
78 -> 89 -0.14780
79 -> 88 0.10806
79 -> 89 -0.22380
79 -> 90 0.11235
79 -> 91 0.16520
79 -> 93 0.12784

Excited State 30: Singlet-A 6.6678 eV 185.94 nm f=0.0371 <S**2>=0.000
67 -> 80 -0.10827
68 -> 80 0.23915
71 -> 80 0.34667
75 -> 80 -0.23558
76 -> 82 0.18016
77 -> 80 -0.13280
77 -> 81 0.15898
79 -> 87 -0.17281
79 -> 90 -0.10939

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.5679 eV 347.49 nm f=1.1442 <S**2>=0.000
77 -> 80 0.23502
78 -> 80 -0.26808
79 -> 80 0.57484
79 -> 81 0.12528
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.00304915
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.9522 eV 313.71 nm f=0.0031 <S**2>=0.000
73 -> 80 0.64279
73 -> 81 -0.12593
73 -> 87 0.14329
74 -> 80 -0.11606

Excited State 3: Singlet-A 4.3559 eV 284.64 nm f=0.0523 <S**2>=0.000
77 -> 80 -0.20986
77 -> 81 -0.16022
78 -> 80 0.15494
78 -> 84 0.23432
79 -> 81 0.55857
79 -> 84 0.11409

Excited State 4: Singlet-A 4.4286 eV 279.96 nm f=0.0441 <S**2>=0.000
77 -> 81 0.12928
78 -> 80 0.38778
78 -> 81 0.45958
79 -> 80 0.20585

79 -> 84 -0.21857

Excited State 5: Singlet-A 4.5114 eV 274.83 nm f=0.0102 <S**2>=0.000
76 -> 80 0.64404
77 -> 82 0.10599
77 -> 83 -0.11627
79 -> 82 0.13199
79 -> 83 -0.13312

Excited State 6: Singlet-A 4.5992 eV 269.58 nm f=0.0005 <S**2>=0.000
70 -> 80 0.66529
70 -> 81 -0.12842
70 -> 87 0.14273

Excited State 7: Singlet-A 4.8218 eV 257.14 nm f=0.0654 <S**2>=0.000
75 -> 80 -0.15981
77 -> 80 0.37710
78 -> 80 -0.24745
78 -> 81 0.29321
79 -> 80 -0.29856
79 -> 81 0.21467
79 -> 87 0.10625

Excited State 8: Singlet-A 4.9764 eV 249.14 nm f=0.0228 <S**2>=0.000
74 -> 80 -0.16615
75 -> 80 -0.14787
77 -> 80 0.37779
78 -> 80 0.40273
78 -> 81 -0.21879
78 -> 87 -0.12927
79 -> 84 0.19448

Excited State 9: Singlet-A 5.1977 eV 238.54 nm f=0.5867 <S**2>=0.000
76 -> 80 0.12732
77 -> 81 -0.14597
78 -> 81 0.26944
78 -> 84 0.19644
78 -> 87 -0.12953
79 -> 81 -0.22179
79 -> 82 -0.25271
79 -> 83 0.11253
79 -> 84 0.31392
79 -> 87 0.12236

Excited State 10: Singlet-A 5.3376 eV 232.28 nm f=0.4517 <S**2>=0.000
76 -> 80 -0.23381
77 -> 82 0.14725
77 -> 83 -0.16414
78 -> 81 0.13378
78 -> 82 -0.18179
78 -> 83 0.15144
78 -> 84 0.11544
79 -> 81 -0.11226
79 -> 82 0.34110
79 -> 83 -0.28080
79 -> 84 0.21401

Excited State 11: Singlet-A 5.5314 eV 224.15 nm f=0.0056 <S**2>=0.000
78 -> 85 -0.10012

79 -> 82 0.37258
79 -> 83 0.43582
79 -> 86 0.20630
79 -> 88 -0.16638

Excited State 12: Singlet-A 5.6704 eV 218.65 nm f=0.1249 <S**2>=0.000
72 -> 80 0.20034
74 -> 80 -0.20956
75 -> 80 -0.19314
75 -> 81 -0.10046
77 -> 80 -0.10687
77 -> 87 -0.14066
78 -> 84 0.32910
79 -> 81 -0.15034
79 -> 84 -0.21109
79 -> 89 0.12369
79 -> 90 0.25237

Excited State 13: Singlet-A 5.7277 eV 216.46 nm f=0.0926 <S**2>=0.000
72 -> 80 0.22831
74 -> 80 -0.17495
75 -> 80 -0.22187
77 -> 80 -0.15356
77 -> 81 0.15121
77 -> 84 -0.11630
78 -> 81 0.13596
78 -> 84 -0.10883
78 -> 90 -0.16820
79 -> 84 0.24664
79 -> 87 -0.22180
79 -> 89 -0.11263
79 -> 90 -0.19003

Excited State 14: Singlet-A 5.8034 eV 213.64 nm f=0.0691 <S**2>=0.000
78 -> 82 0.23401
78 -> 83 0.23648
78 -> 84 -0.13746
78 -> 85 -0.16858
78 -> 87 0.18389
78 -> 89 0.13370
78 -> 90 0.21786
79 -> 84 0.20725
79 -> 85 -0.21790
79 -> 87 0.12253
79 -> 90 0.22409

Excited State 15: Singlet-A 5.8105 eV 213.38 nm f=0.0544 <S**2>=0.000
78 -> 82 -0.25563
78 -> 83 -0.22604
78 -> 84 -0.22605
78 -> 87 0.15868
78 -> 88 0.11164
78 -> 90 0.17149
79 -> 84 0.15370
79 -> 85 0.29718
79 -> 89 0.13172
79 -> 90 0.19539

Excited State 16: Singlet-A 5.8843 eV 210.71 nm f=0.2486 <S**2>=0.000

74 -> 80 -0.17635
75 -> 80 -0.18731
77 -> 80 -0.14577
77 -> 81 -0.19083
77 -> 87 0.10899
78 -> 84 -0.22420
78 -> 87 -0.10004
79 -> 84 -0.11155
79 -> 86 -0.12915
79 -> 87 0.37723
79 -> 90 -0.18373

Excited State 17: Singlet-A 6.0595 eV 204.61 nm f=0.2743 <S**2>=0.000
75 -> 84 0.12223
77 -> 81 0.15733
77 -> 90 0.15909
78 -> 82 -0.10473
78 -> 84 0.22437
78 -> 87 0.10282
78 -> 88 0.12465
78 -> 89 0.19862
78 -> 90 0.31463
79 -> 86 -0.20664
79 -> 89 -0.13131
79 -> 90 -0.20432

Excited State 18: Singlet-A 6.0849 eV 203.76 nm f=0.0368 <S**2>=0.000
78 -> 85 0.18780
78 -> 86 0.11029
78 -> 87 0.11133
78 -> 90 0.17665
79 -> 83 -0.13231
79 -> 86 0.47155
79 -> 88 -0.11601
79 -> 90 -0.12643

Excited State 19: Singlet-A 6.1616 eV 201.22 nm f=0.0093 <S**2>=0.000
77 -> 81 -0.10462
77 -> 82 0.15404
77 -> 83 0.14721
78 -> 82 0.19094
78 -> 83 0.16006
78 -> 85 -0.16161
78 -> 88 -0.17919
78 -> 89 0.10435
79 -> 85 0.43757
79 -> 86 -0.10023

Excited State 20: Singlet-A 6.1746 eV 200.80 nm f=0.1260 <S**2>=0.000
71 -> 80 0.64980
79 -> 83 -0.10420

Excited State 21: Singlet-A 6.2110 eV 199.62 nm f=0.1969 <S**2>=0.000
71 -> 80 0.13372
75 -> 80 0.11234
77 -> 81 0.45682
78 -> 81 -0.10495
78 -> 87 -0.11252
78 -> 88 -0.10923

79 -> 85 0.10820
79 -> 87 0.28043

Excited State 22: Singlet-A 6.2475 eV 198.45 nm f=0.0100 <S**2>=0.000
77 -> 82 -0.12269
78 -> 85 0.35750
78 -> 86 -0.14927
78 -> 88 -0.15535
78 -> 89 0.16215
79 -> 86 -0.20642
79 -> 88 -0.32148
79 -> 89 0.15747
79 -> 94 -0.10434
79 -> 97 0.10100

Excited State 23: Singlet-A 6.3595 eV 194.96 nm f=0.0046 <S**2>=0.000
78 -> 86 0.46542
78 -> 87 0.12550
79 -> 86 -0.12947
79 -> 89 -0.29244
79 -> 90 0.17025
79 -> 91 0.14771

Excited State 24: Singlet-A 6.4093 eV 193.44 nm f=0.0179 <S**2>=0.000
74 -> 80 -0.27452
74 -> 81 -0.29650
75 -> 80 0.20110
75 -> 81 0.40770
78 -> 87 -0.10491
79 -> 87 -0.12686

Excited State 25: Singlet-A 6.4753 eV 191.47 nm f=0.0016 <S**2>=0.000
77 -> 82 0.10708
77 -> 83 -0.10513
77 -> 85 0.20736
78 -> 85 0.23132
78 -> 88 -0.28019
79 -> 83 0.20947
79 -> 88 0.33576
79 -> 93 0.14542

Excited State 26: Singlet-A 6.4951 eV 190.89 nm f=0.0055 <S**2>=0.000
74 -> 81 -0.16605
75 -> 81 0.10066
75 -> 82 -0.10622
75 -> 83 0.10587
76 -> 82 -0.12035
76 -> 83 0.11913
76 -> 87 -0.13276
77 -> 81 -0.14438
77 -> 82 0.20218
77 -> 83 -0.16754
78 -> 83 0.10977
79 -> 82 -0.16387
79 -> 83 0.14842
79 -> 88 -0.17117
79 -> 89 -0.11294
79 -> 93 -0.19004
79 -> 94 0.10465

Excited State 27: Singlet-A 6.5245 eV 190.03 nm f=0.1005 <S**2>=0.000
75 -> 83 0.11381
76 -> 81 0.11584
76 -> 82 0.22417
76 -> 83 -0.20303
77 -> 82 0.13654
77 -> 83 -0.18709
77 -> 85 -0.10442
78 -> 86 0.11001
79 -> 82 -0.15901
79 -> 83 0.10911
79 -> 88 -0.10646
79 -> 89 0.12614
79 -> 91 0.10659
79 -> 92 0.14266
79 -> 93 0.15368
79 -> 94 -0.17916

Excited State 28: Singlet-A 6.6222 eV 187.22 nm f=0.0189 <S**2>=0.000
75 -> 81 -0.14531
77 -> 82 0.10770
77 -> 83 -0.10913
78 -> 82 0.27953
78 -> 83 -0.23897
78 -> 87 -0.25078
78 -> 89 0.13417
78 -> 90 0.12381
79 -> 87 -0.15372
79 -> 91 -0.15827
79 -> 92 -0.10416

Excited State 29: Singlet-A 6.6572 eV 186.24 nm f=0.1738 <S**2>=0.000
72 -> 80 -0.19573
76 -> 82 -0.26666
76 -> 83 0.31529
77 -> 80 -0.10814
77 -> 86 0.10083
78 -> 86 0.12730
78 -> 89 -0.17072
79 -> 89 0.23349
79 -> 92 0.18124

Excited State 30: Singlet-A 6.6668 eV 185.97 nm f=0.0023 <S**2>=0.000
66 -> 80 0.15099
68 -> 80 0.26116
72 -> 80 0.29057
75 -> 80 0.19416
75 -> 81 -0.10474
77 -> 80 0.11856
77 -> 81 -0.13982
77 -> 86 0.10652
78 -> 82 0.11551
78 -> 83 -0.10633
79 -> 89 0.13558
79 -> 90 -0.14042
79 -> 92 0.10698

Single-point TDDFT B3LYP/Def2TZVPD/PCM(DMSO) over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometry

1

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7468 eV 451.38 nm f=0.2146 <S**2>=0.000
79 -> 80 0.70588
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.60372281
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1496 eV 393.65 nm f=0.4537 <S**2>=0.000
78 -> 80 0.70307

Excited State 3: Singlet-A 3.8259 eV 324.06 nm f=0.0000 <S**2>=0.000
73 -> 80 0.18591
74 -> 80 0.66996

Excited State 4: Singlet-A 3.9796 eV 311.55 nm f=0.3338 <S**2>=0.000
77 -> 80 -0.41731
79 -> 81 0.54815

Excited State 5: Singlet-A 4.0736 eV 304.36 nm f=0.1284 <S**2>=0.000
76 -> 80 0.10505
77 -> 80 0.54764
79 -> 81 0.39980
79 -> 83 0.10209

Excited State 6: Singlet-A 4.1411 eV 299.40 nm f=0.0076 <S**2>=0.000
76 -> 80 0.65543
78 -> 82 -0.11974
79 -> 82 -0.14073

Excited State 7: Singlet-A 4.1959 eV 295.49 nm f=0.0420 <S**2>=0.000
78 -> 81 0.58929
79 -> 81 -0.10802
79 -> 82 0.10694
79 -> 83 0.31337
79 -> 84 -0.12307

Excited State 8: Singlet-A 4.4558 eV 278.25 nm f=0.0004 <S**2>=0.000
70 -> 80 0.67017
73 -> 80 0.18045

Excited State 9: Singlet-A 4.4868 eV 276.33 nm f=0.0484 <S**2>=0.000
76 -> 80 0.16913
78 -> 81 -0.10540
78 -> 82 0.11932
79 -> 82 0.66145

Excited State 10: Singlet-A 4.7245 eV 262.43 nm f=0.0040 <S**2>=0.000
75 -> 80 0.69176

Excited State 11: Singlet-A 4.8301 eV 256.69 nm f=0.6244 <S**2>=0.000

77 -> 81 -0.22887
78 -> 81 -0.29719
78 -> 82 0.21622
78 -> 84 0.11873
79 -> 83 0.51884

Excited State 12: Singlet-A 4.8976 eV 253.15 nm f=0.2231 <S**2>=0.000
78 -> 81 0.10629
78 -> 82 0.63390
79 -> 82 -0.13235
79 -> 83 -0.17302

Excited State 13: Singlet-A 4.9956 eV 248.18 nm f=0.0002 <S**2>=0.000
70 -> 80 -0.18300
73 -> 80 0.64906
74 -> 80 -0.18168

Excited State 14: Singlet-A 5.1330 eV 241.54 nm f=0.0015 <S**2>=0.000
75 -> 81 -0.11244
77 -> 81 0.36831
79 -> 83 0.17795
79 -> 84 0.52607
79 -> 86 -0.13995

Excited State 15: Singlet-A 5.2690 eV 235.31 nm f=0.0001 <S**2>=0.000
79 -> 85 0.65649
79 -> 87 0.22504

Excited State 16: Singlet-A 5.2839 eV 234.65 nm f=0.0627 <S**2>=0.000
75 -> 81 0.12093
77 -> 81 0.30606
78 -> 83 0.50600
79 -> 83 0.10654
79 -> 84 -0.20316
79 -> 86 0.24964

Excited State 17: Singlet-A 5.3676 eV 230.99 nm f=0.0035 <S**2>=0.000
72 -> 80 -0.16357
75 -> 81 0.19191
78 -> 83 -0.23777
79 -> 84 0.21269
79 -> 86 0.56127

Excited State 18: Singlet-A 5.4636 eV 226.93 nm f=0.0166 <S**2>=0.000
72 -> 80 0.66714
77 -> 81 0.10127
78 -> 83 -0.10355
79 -> 86 0.13517

Excited State 19: Singlet-A 5.5504 eV 223.38 nm f=0.0003 <S**2>=0.000
78 -> 85 -0.33080
79 -> 85 -0.15177
79 -> 87 0.53525
79 -> 88 -0.24207

Excited State 20: Singlet-A 5.5877 eV 221.89 nm f=0.0350 <S**2>=0.000
75 -> 83 0.11596
78 -> 84 0.62694
78 -> 86 -0.20100

Excited State 21: Singlet-A 5.6441 eV 219.67 nm f=0.2115 <S**2>=0.000
76 -> 81 0.22496
76 -> 84 -0.12303
77 -> 81 -0.20162
77 -> 82 0.50883
78 -> 83 0.20896
79 -> 84 0.14188

Excited State 22: Singlet-A 5.7059 eV 217.29 nm f=0.0005 <S**2>=0.000
78 -> 85 0.58450
79 -> 85 -0.10973
79 -> 87 0.23595
79 -> 88 -0.23284

Excited State 23: Singlet-A 5.7285 eV 216.43 nm f=0.5058 <S**2>=0.000
76 -> 81 0.37602
77 -> 81 0.33518
77 -> 82 0.18975
78 -> 83 -0.28063
79 -> 83 0.12986
79 -> 84 -0.23355
79 -> 86 -0.10589

Excited State 24: Singlet-A 5.7938 eV 214.00 nm f=0.1524 <S**2>=0.000
75 -> 81 -0.24176
75 -> 83 -0.12065
78 -> 83 -0.10034
78 -> 84 0.22102
78 -> 86 0.54546
79 -> 84 -0.11251
79 -> 86 0.11767

Excited State 25: Singlet-A 5.8078 eV 213.48 nm f=0.0012 <S**2>=0.000
79 -> 87 0.21584
79 -> 88 0.48687
79 -> 89 -0.40423
79 -> 90 0.16279

Excited State 26: Singlet-A 5.8726 eV 211.12 nm f=0.0626 <S**2>=0.000
71 -> 80 0.34565
76 -> 81 0.47349
77 -> 81 -0.11006
77 -> 82 -0.27448
78 -> 83 0.10680
78 -> 86 0.14466
79 -> 84 0.10419

Excited State 27: Singlet-A 5.8951 eV 210.32 nm f=0.0004 <S**2>=0.000
78 -> 87 0.30382
79 -> 85 -0.11199
79 -> 87 0.19273
79 -> 88 0.26595
79 -> 89 0.49605
79 -> 92 0.14404

Excited State 28: Singlet-A 5.9579 eV 208.10 nm f=0.0244 <S**2>=0.000
71 -> 80 -0.30369
75 -> 81 0.51624

78 -> 86 0.25590
79 -> 86 -0.17243

Excited State 29: Singlet-A 5.9818 eV 207.27 nm f=0.0000 <S**2>=0.000
73 -> 81 0.64952
74 -> 81 -0.22089

Excited State 30: Singlet-A 5.9835 eV 207.21 nm f=0.0487 <S**2>=0.000
71 -> 80 0.50279
75 -> 81 0.28656
76 -> 81 -0.24349
77 -> 82 0.23894

1-

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4769 eV 500.57 nm f=0.9450 <S**2>=0.000
79 -> 80 0.70422
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.14571407
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9952 eV 413.94 nm f=0.2088 <S**2>=0.000
78 -> 80 0.69855

Excited State 3: Singlet-A 3.5887 eV 345.48 nm f=0.2625 <S**2>=0.000
77 -> 80 0.24036
79 -> 81 0.64929

Excited State 4: Singlet-A 3.7409 eV 331.43 nm f=0.0000 <S**2>=0.000
72 -> 80 0.57885
73 -> 80 0.18067
76 -> 80 -0.34171

Excited State 5: Singlet-A 3.8635 eV 320.91 nm f=0.0699 <S**2>=0.000
77 -> 80 0.63574
78 -> 83 -0.10526
79 -> 81 -0.20526
79 -> 83 0.15781

Excited State 6: Singlet-A 3.9946 eV 310.38 nm f=0.0001 <S**2>=0.000
72 -> 80 0.32747
76 -> 80 0.61217

Excited State 7: Singlet-A 4.0050 eV 309.58 nm f=0.0050 <S**2>=0.000
75 -> 80 0.53707
79 -> 82 -0.43810

Excited State 8: Singlet-A 4.1141 eV 301.36 nm f=0.0039 <S**2>=0.000
75 -> 80 -0.34457
78 -> 81 0.42160
79 -> 82 -0.38327
79 -> 83 -0.17438

Excited State 9: Singlet-A 4.1721 eV 297.18 nm f=0.0671 <S**2>=0.000
75 -> 80 0.27850
78 -> 81 0.42697
79 -> 82 0.37653

79 -> 83 -0.28238

Excited State 10: Singlet-A 4.4781 eV 276.87 nm f=0.0001 <S**2>=0.000
69 -> 80 0.52853
72 -> 80 0.13583
73 -> 80 -0.43428

Excited State 11: Singlet-A 4.4905 eV 276.10 nm f=0.4032 <S**2>=0.000
77 -> 80 -0.12621
77 -> 81 0.11186
78 -> 81 0.32759
79 -> 83 0.56650
79 -> 85 0.12696

Excited State 12: Singlet-A 4.6056 eV 269.20 nm f=0.0008 <S**2>=0.000
69 -> 80 0.44899
72 -> 80 -0.14523
73 -> 80 0.51205

Excited State 13: Singlet-A 4.6430 eV 267.04 nm f=0.0003 <S**2>=0.000
79 -> 84 0.68769
79 -> 88 0.10166

Excited State 14: Singlet-A 4.7030 eV 263.63 nm f=0.0110 <S**2>=0.000
74 -> 80 0.59665
77 -> 81 -0.10314
79 -> 85 0.33437

Excited State 15: Singlet-A 4.7853 eV 259.10 nm f=0.0341 <S**2>=0.000
74 -> 80 0.11580
77 -> 81 0.46609
78 -> 82 -0.26904
78 -> 83 -0.37032
79 -> 83 -0.15811

Excited State 16: Singlet-A 4.8529 eV 255.48 nm f=0.0244 <S**2>=0.000
74 -> 80 -0.34302
78 -> 81 -0.10182
79 -> 85 0.56513
79 -> 87 -0.12568

Excited State 17: Singlet-A 4.9433 eV 250.81 nm f=0.0053 <S**2>=0.000
78 -> 84 -0.14036
79 -> 86 0.67802

Excited State 18: Singlet-A 4.9866 eV 248.63 nm f=0.0611 <S**2>=0.000
77 -> 81 0.13323
78 -> 82 0.62449
78 -> 83 -0.22827
79 -> 87 -0.13768

Excited State 19: Singlet-A 5.0329 eV 246.35 nm f=0.0500 <S**2>=0.000
71 -> 80 -0.15692
78 -> 83 -0.18357
79 -> 87 0.62988

Excited State 20: Singlet-A 5.1511 eV 240.69 nm f=0.0011 <S**2>=0.000
78 -> 84 0.14444
78 -> 86 0.12011

79 -> 88 0.65759
79 -> 89 -0.10257

Excited State 21: Singlet-A 5.2459 eV 236.34 nm f=0.0001 <S**2>=0.000
79 -> 88 0.10178
79 -> 89 0.66840

Excited State 22: Singlet-A 5.2475 eV 236.27 nm f=0.0508 <S**2>=0.000
71 -> 80 0.62624
77 -> 81 -0.15968
78 -> 83 -0.15830
78 -> 85 -0.14187
79 -> 87 0.13312

Excited State 23: Singlet-A 5.2865 eV 234.53 nm f=0.0007 <S**2>=0.000
78 -> 84 0.60367
78 -> 86 0.25696
79 -> 86 0.12946
79 -> 88 -0.16785

Excited State 24: Singlet-A 5.3301 eV 232.61 nm f=0.0104 <S**2>=0.000
71 -> 80 0.19872
74 -> 81 -0.15940
78 -> 83 0.13280
78 -> 85 0.60452
78 -> 87 -0.17414

Excited State 25: Singlet-A 5.3827 eV 230.34 nm f=0.0002 <S**2>=0.000
76 -> 81 0.68575

Excited State 26: Singlet-A 5.4800 eV 226.25 nm f=0.0000 <S**2>=0.000
78 -> 88 0.14047
79 -> 89 0.10191
79 -> 90 0.66488

Excited State 27: Singlet-A 5.5510 eV 223.35 nm f=0.7722 <S**2>=0.000
71 -> 80 0.14449
74 -> 81 0.13175
77 -> 81 0.39765
77 -> 82 0.20049
78 -> 83 0.40316
78 -> 87 0.11216
79 -> 85 0.12599
79 -> 87 0.15970

Excited State 28: Singlet-A 5.6020 eV 221.32 nm f=0.0004 <S**2>=0.000
78 -> 84 -0.18419
78 -> 86 0.51113
78 -> 88 -0.28901
78 -> 89 -0.18313
79 -> 90 0.14392
79 -> 91 0.20100

Excited State 29: Singlet-A 5.6290 eV 220.26 nm f=0.0094 <S**2>=0.000
75 -> 81 0.52253
77 -> 82 -0.41027
78 -> 87 0.10046

Excited State 30: Singlet-A 5.6697 eV 218.68 nm f=0.0003 <S**2>=0.000

72 -> 81 -0.12289
73 -> 81 0.67387

1’

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7053 eV 458.30 nm f=0.3570 <S**2>=0.000
79 -> 80 0.70629
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.60277803
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1639 eV 391.88 nm f=0.3631 <S**2>=0.000
78 -> 80 0.70257

Excited State 3: Singlet-A 3.8232 eV 324.29 nm f=0.0000 <S**2>=0.000
74 -> 80 0.69460

Excited State 4: Singlet-A 3.9214 eV 316.17 nm f=0.3638 <S**2>=0.000
77 -> 80 -0.25916
79 -> 81 0.63556

Excited State 5: Singlet-A 4.0463 eV 306.42 nm f=0.0825 <S**2>=0.000
77 -> 80 0.63994
79 -> 81 0.24056
79 -> 83 0.10909

Excited State 6: Singlet-A 4.1516 eV 298.64 nm f=0.0069 <S**2>=0.000
76 -> 80 0.63772
78 -> 82 -0.12305
79 -> 82 -0.22621

Excited State 7: Singlet-A 4.2161 eV 294.07 nm f=0.0263 <S**2>=0.000
78 -> 81 0.58078
79 -> 81 -0.10802
79 -> 83 0.33265
79 -> 84 -0.13414

Excited State 8: Singlet-A 4.4144 eV 280.86 nm f=0.0178 <S**2>=0.000
76 -> 80 0.24571
79 -> 82 0.65124

Excited State 9: Singlet-A 4.4625 eV 277.84 nm f=0.0005 <S**2>=0.000
70 -> 80 0.69454

Excited State 10: Singlet-A 4.7396 eV 261.59 nm f=0.0025 <S**2>=0.000
75 -> 80 0.69648

Excited State 11: Singlet-A 4.7718 eV 259.83 nm f=0.6954 <S**2>=0.000
77 -> 81 -0.20987
78 -> 81 -0.34029
78 -> 82 0.16245
78 -> 84 0.10845
79 -> 83 0.52411

Excited State 12: Singlet-A 4.9001 eV 253.03 nm f=0.0870 <S**2>=0.000
78 -> 82 0.65002
79 -> 82 -0.10464

79 -> 83 -0.16904
79 -> 84 -0.11309

Excited State 13: Singlet-A 5.0797 eV 244.08 nm f=0.0025 <S**2>=0.000
77 -> 81 0.41355
78 -> 82 0.11201
79 -> 83 0.16716
79 -> 84 0.48447
79 -> 86 -0.11481

Excited State 14: Singlet-A 5.1461 eV 240.93 nm f=0.0002 <S**2>=0.000
73 -> 80 0.69701

Excited State 15: Singlet-A 5.1814 eV 239.29 nm f=0.0004 <S**2>=0.000
79 -> 85 0.66800
79 -> 87 0.16893

Excited State 16: Singlet-A 5.2512 eV 236.11 nm f=0.0387 <S**2>=0.000
75 -> 81 0.11815
77 -> 81 0.28878
78 -> 83 0.46944
79 -> 83 0.10132
79 -> 84 -0.24287
79 -> 86 0.30642

Excited State 17: Singlet-A 5.3356 eV 232.37 nm f=0.0171 <S**2>=0.000
72 -> 80 -0.13939
75 -> 81 0.16308
78 -> 83 -0.26607
79 -> 84 0.22542
79 -> 86 0.55773

Excited State 18: Singlet-A 5.4684 eV 226.73 nm f=0.0154 <S**2>=0.000
72 -> 80 0.67086
78 -> 83 -0.11889
79 -> 86 0.11192

Excited State 19: Singlet-A 5.4936 eV 225.69 nm f=0.0010 <S**2>=0.000
78 -> 85 -0.24010
79 -> 85 -0.10829
79 -> 87 0.60801
79 -> 88 -0.19245

Excited State 20: Singlet-A 5.5994 eV 221.42 nm f=0.0447 <S**2>=0.000
75 -> 83 0.12031
77 -> 83 -0.13303
78 -> 84 0.60015
78 -> 86 -0.20344
79 -> 84 0.12790

Excited State 21: Singlet-A 5.6311 eV 220.18 nm f=0.1965 <S**2>=0.000
76 -> 81 0.22343
76 -> 83 -0.10367
76 -> 84 -0.11238
77 -> 81 -0.19293
77 -> 82 0.52373
78 -> 83 0.19053
79 -> 84 0.15359

Excited State 22: Singlet-A 5.7204 eV 216.74 nm f=0.0006 <S**2>=0.000
78 -> 85 0.62298
79 -> 87 0.21507
79 -> 89 -0.14345

Excited State 23: Singlet-A 5.7408 eV 215.97 nm f=0.6084 <S**2>=0.000
76 -> 81 0.33750
77 -> 81 0.33602
77 -> 82 0.18794
78 -> 83 -0.31451
78 -> 84 0.10346
78 -> 86 -0.11614
79 -> 84 -0.23397

Excited State 24: Singlet-A 5.7617 eV 215.19 nm f=0.0000 <S**2>=0.000
79 -> 85 -0.10220
79 -> 87 0.10518
79 -> 88 0.58150
79 -> 89 -0.27858
79 -> 90 0.21279

Excited State 25: Singlet-A 5.8069 eV 213.51 nm f=0.1099 <S**2>=0.000
75 -> 81 -0.33281
78 -> 84 0.24217
78 -> 86 0.50187
79 -> 86 0.14555

Excited State 26: Singlet-A 5.8725 eV 211.13 nm f=0.0010 <S**2>=0.000
78 -> 87 0.23630
79 -> 87 0.15389
79 -> 88 0.20532
79 -> 89 0.57452
79 -> 92 -0.14721

Excited State 27: Singlet-A 5.8753 eV 211.03 nm f=0.1011 <S**2>=0.000
71 -> 80 0.40076
76 -> 81 0.46756
77 -> 81 -0.11415
77 -> 82 -0.23274
78 -> 83 0.12145

Excited State 28: Singlet-A 5.9692 eV 207.71 nm f=0.0614 <S**2>=0.000
71 -> 80 0.54665
76 -> 81 -0.30465
77 -> 82 0.25377

Excited State 29: Singlet-A 5.9917 eV 206.93 nm f=0.0051 <S**2>=0.000
75 -> 81 0.55175
78 -> 86 0.35984
79 -> 86 -0.14375

Excited State 30: Singlet-A 5.9938 eV 206.85 nm f=0.0000 <S**2>=0.000
78 -> 87 0.29651
78 -> 88 -0.22405
79 -> 88 -0.21227
79 -> 90 0.52929

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4527 eV 505.50 nm f=0.9932 <S**2>=0.000
79 -> 80 0.70445
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.14373970
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0227 eV 410.18 nm f=0.1388 <S**2>=0.000
78 -> 80 0.69456
79 -> 81 0.11485

Excited State 3: Singlet-A 3.5103 eV 353.20 nm f=0.2758 <S**2>=0.000
77 -> 80 0.36736
79 -> 81 0.58315

Excited State 4: Singlet-A 3.6988 eV 335.20 nm f=0.0293 <S**2>=0.000
72 -> 80 0.27487
74 -> 80 -0.11724
75 -> 80 -0.10087
76 -> 80 0.20171
77 -> 80 0.46746
79 -> 81 -0.32407
79 -> 83 -0.10702

Excited State 5: Singlet-A 3.7805 eV 327.95 nm f=0.0149 <S**2>=0.000
72 -> 80 0.57056
74 -> 80 -0.13295
76 -> 80 0.10675
77 -> 80 -0.31350
79 -> 81 0.12644

Excited State 6: Singlet-A 3.9913 eV 310.64 nm f=0.0007 <S**2>=0.000
75 -> 80 -0.30834
76 -> 80 -0.18919
79 -> 82 0.59585

Excited State 7: Singlet-A 4.1042 eV 302.09 nm f=0.0238 <S**2>=0.000
72 -> 80 -0.12592
75 -> 80 0.15679
76 -> 80 0.41482
78 -> 81 0.30559
79 -> 82 0.21521
79 -> 83 0.35318

Excited State 8: Singlet-A 4.1388 eV 299.57 nm f=0.0197 <S**2>=0.000
75 -> 80 0.45703
76 -> 80 0.16206
78 -> 81 -0.31617
79 -> 82 0.28604
79 -> 83 -0.25451

Excited State 9: Singlet-A 4.1977 eV 295.36 nm f=0.0032 <S**2>=0.000
72 -> 80 -0.19798
75 -> 80 -0.37365
76 -> 80 0.40943
77 -> 80 -0.14338
78 -> 81 -0.31978

Excited State 10: Singlet-A 4.4357 eV 279.51 nm f=0.3918 <S**2>=0.000
76 -> 80 -0.12476
77 -> 80 0.12559
77 -> 81 -0.10331
78 -> 81 -0.40270
79 -> 83 0.49183
79 -> 84 0.13834
79 -> 85 -0.11630

Excited State 11: Singlet-A 4.5229 eV 274.13 nm f=0.0007 <S**2>=0.000
69 -> 80 0.69215

Excited State 12: Singlet-A 4.5779 eV 270.83 nm f=0.0085 <S**2>=0.000
79 -> 84 0.63550
79 -> 85 0.24166
79 -> 88 0.13631

Excited State 13: Singlet-A 4.6942 eV 264.12 nm f=0.0128 <S**2>=0.000
73 -> 80 0.34435
74 -> 80 0.28432
77 -> 81 -0.30102
78 -> 81 -0.10166
78 -> 83 -0.12135
79 -> 85 0.38768

Excited State 14: Singlet-A 4.7042 eV 263.56 nm f=0.0036 <S**2>=0.000
73 -> 80 0.60658
74 -> 80 -0.18016
77 -> 81 0.15904
79 -> 85 -0.20136

Excited State 15: Singlet-A 4.7553 eV 260.73 nm f=0.0116 <S**2>=0.000
74 -> 80 0.28113
77 -> 81 0.42666
78 -> 83 0.32986
79 -> 83 0.15105
79 -> 85 0.17727
79 -> 87 0.18396

Excited State 16: Singlet-A 4.8589 eV 255.17 nm f=0.0083 <S**2>=0.000
74 -> 80 0.50143
79 -> 84 0.13536
79 -> 85 -0.35937
79 -> 87 -0.22147

Excited State 17: Singlet-A 4.8900 eV 253.55 nm f=0.0046 <S**2>=0.000
78 -> 84 -0.12298
79 -> 86 0.67701

Excited State 18: Singlet-A 4.9598 eV 249.98 nm f=0.0281 <S**2>=0.000
78 -> 82 0.58042
79 -> 87 -0.36059

Excited State 19: Singlet-A 4.9808 eV 248.93 nm f=0.0532 <S**2>=0.000
71 -> 80 -0.10573
78 -> 82 0.36123
78 -> 83 -0.21942
79 -> 85 -0.17560
79 -> 87 0.48543

Excited State 20: Singlet-A 5.1232 eV 242.00 nm f=0.0024 <S**2>=0.000
79 -> 84 -0.12523
79 -> 88 0.66357
79 -> 89 0.12340

Excited State 21: Singlet-A 5.2100 eV 237.97 nm f=0.0089 <S**2>=0.000
78 -> 86 -0.10530
79 -> 88 -0.11132
79 -> 89 0.67039

Excited State 22: Singlet-A 5.2356 eV 236.81 nm f=0.3583 <S**2>=0.000
71 -> 80 0.38341
75 -> 81 -0.13540
76 -> 81 0.28506
77 -> 81 0.30348
78 -> 83 -0.33916

Excited State 23: Singlet-A 5.3184 eV 233.12 nm f=0.0015 <S**2>=0.000
78 -> 84 0.60694
78 -> 85 0.13029
78 -> 86 0.22051
79 -> 86 0.12939

Excited State 24: Singlet-A 5.3390 eV 232.22 nm f=0.0478 <S**2>=0.000
71 -> 80 0.40856
75 -> 81 0.11117
76 -> 81 -0.30296
77 -> 81 -0.10404
77 -> 82 0.12969
78 -> 85 0.34305
78 -> 87 0.12131
79 -> 87 0.14909

Excited State 25: Singlet-A 5.3611 eV 231.26 nm f=0.0172 <S**2>=0.000
71 -> 80 -0.35710
74 -> 81 -0.13161
78 -> 83 -0.20041
78 -> 85 0.49835
78 -> 87 0.12294

Excited State 26: Singlet-A 5.4223 eV 228.65 nm f=0.0007 <S**2>=0.000
79 -> 90 0.67789

Excited State 27: Singlet-A 5.4690 eV 226.71 nm f=0.0046 <S**2>=0.000
75 -> 81 -0.21662
76 -> 82 0.16374
77 -> 82 0.60850

Excited State 28: Singlet-A 5.6024 eV 221.31 nm f=0.0092 <S**2>=0.000
78 -> 84 -0.12027
78 -> 86 0.48522
78 -> 87 -0.11447
78 -> 88 -0.23660
78 -> 89 0.11117
79 -> 91 0.33604

Excited State 29: Singlet-A 5.6503 eV 219.43 nm f=0.0648 <S**2>=0.000
74 -> 81 -0.14147

76 -> 81 0.22886
78 -> 83 0.19466
78 -> 87 0.52669
79 -> 91 0.23951

Excited State 30: Singlet-A 5.6798 eV 218.29 nm f=0.0125 <S**2>=0.000
78 -> 84 0.16344
78 -> 86 -0.34281
78 -> 87 -0.14074
79 -> 91 0.52865

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8626 eV 433.12 nm f=0.3315 <S**2>=0.000
79 -> 80 0.69853
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.59305938
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1067 eV 399.09 nm f=0.1722 <S**2>=0.000
78 -> 80 0.69879

Excited State 3: Singlet-A 3.7888 eV 327.24 nm f=0.2665 <S**2>=0.000
73 -> 80 0.39180
74 -> 80 0.13871
75 -> 80 0.14014
77 -> 80 0.52414
79 -> 81 -0.13347

Excited State 4: Singlet-A 3.8368 eV 323.15 nm f=0.1437 <S**2>=0.000
73 -> 80 0.52376
74 -> 80 0.12132
77 -> 80 -0.41930
79 -> 81 0.10982

Excited State 5: Singlet-A 4.0683 eV 304.75 nm f=0.1431 <S**2>=0.000
76 -> 80 -0.23157
77 -> 80 0.15414
78 -> 81 -0.18487
78 -> 83 -0.17272
79 -> 81 0.56764
79 -> 83 -0.13554

Excited State 6: Singlet-A 4.0923 eV 302.97 nm f=0.0384 <S**2>=0.000
76 -> 80 0.63729
79 -> 81 0.19200
79 -> 82 -0.12143

Excited State 7: Singlet-A 4.2534 eV 291.49 nm f=0.0548 <S**2>=0.000
78 -> 81 0.60826
79 -> 81 0.25884
79 -> 83 0.21918

Excited State 8: Singlet-A 4.4660 eV 277.62 nm f=0.0005 <S**2>=0.000
71 -> 80 0.69101

Excited State 9: Singlet-A 4.5689 eV 271.36 nm f=0.0114 <S**2>=0.000

76 -> 80 0.15019
78 -> 82 -0.21334
79 -> 82 0.64414

Excited State 10: Singlet-A 4.6702 eV 265.48 nm f=0.0302 <S**2>=0.000
73 -> 80 -0.19525
74 -> 80 0.20865
75 -> 80 0.60706
79 -> 83 0.10304

Excited State 11: Singlet-A 4.8063 eV 257.96 nm f=0.3854 <S**2>=0.000
75 -> 80 0.11680
77 -> 81 0.44540
78 -> 81 0.21127
78 -> 83 -0.16582
78 -> 84 -0.13766
79 -> 81 -0.10914
79 -> 83 -0.38945

Excited State 12: Singlet-A 4.9191 eV 252.05 nm f=0.0025 <S**2>=0.000
74 -> 80 0.11368
78 -> 82 0.64631
79 -> 82 0.22948

Excited State 13: Singlet-A 4.9355 eV 251.21 nm f=0.0025 <S**2>=0.000
73 -> 80 -0.10899
74 -> 80 0.62188
75 -> 80 -0.26119
78 -> 82 -0.12089

Excited State 14: Singlet-A 5.0446 eV 245.78 nm f=0.2320 <S**2>=0.000
77 -> 81 -0.38156
78 -> 83 0.16294
79 -> 83 -0.34892
79 -> 84 0.42434

Excited State 15: Singlet-A 5.1848 eV 239.13 nm f=0.0528 <S**2>=0.000
78 -> 81 -0.10656
78 -> 83 -0.39644
79 -> 83 0.29372
79 -> 84 0.45822

Excited State 16: Singlet-A 5.3320 eV 232.53 nm f=0.0034 <S**2>=0.000
78 -> 84 0.10913
79 -> 85 0.66962
79 -> 87 -0.10223

Excited State 17: Singlet-A 5.3469 eV 231.88 nm f=0.1150 <S**2>=0.000
75 -> 81 0.10104
77 -> 81 0.10819
78 -> 84 0.62265
78 -> 86 -0.10360
79 -> 83 -0.11081
79 -> 84 0.11949
79 -> 85 -0.10077
79 -> 86 -0.14955

Excited State 18: Singlet-A 5.3888 eV 230.08 nm f=0.0671 <S**2>=0.000
74 -> 81 0.16622

77 -> 81 0.10901
78 -> 84 0.14276
78 -> 86 0.11136
79 -> 84 0.12892
79 -> 86 0.61702

Excited State 19: Singlet-A 5.4285 eV 228.39 nm f=0.5593 <S**2>=0.000
75 -> 81 0.26047
77 -> 81 0.30529
78 -> 83 0.42174
78 -> 84 -0.16677
78 -> 86 -0.15734
79 -> 81 0.10570
79 -> 83 0.13652
79 -> 84 0.18596

Excited State 20: Singlet-A 5.4517 eV 227.42 nm f=0.0146 <S**2>=0.000
76 -> 81 0.16172
76 -> 84 -0.16644
77 -> 82 0.63456

Excited State 21: Singlet-A 5.5629 eV 222.88 nm f=0.0036 <S**2>=0.000
78 -> 85 0.60921
78 -> 87 -0.19917
79 -> 87 -0.26060

Excited State 22: Singlet-A 5.5971 eV 221.51 nm f=0.0872 <S**2>=0.000
70 -> 80 -0.23773
74 -> 81 0.16362
78 -> 86 0.56956
79 -> 86 -0.18915

Excited State 23: Singlet-A 5.6152 eV 220.80 nm f=0.0349 <S**2>=0.000
70 -> 80 0.62877
78 -> 86 0.20912

Excited State 24: Singlet-A 5.7537 eV 215.49 nm f=0.0065 <S**2>=0.000
76 -> 81 0.31413
78 -> 85 0.23250
78 -> 88 0.12837
79 -> 87 0.51914
79 -> 88 0.16224

Excited State 25: Singlet-A 5.7548 eV 215.44 nm f=0.0154 <S**2>=0.000
76 -> 81 0.59769
77 -> 82 -0.13014
78 -> 85 -0.13002
79 -> 87 -0.27222

Excited State 26: Singlet-A 5.8994 eV 210.16 nm f=0.0032 <S**2>=0.000
77 -> 85 0.13422
78 -> 85 0.12392
78 -> 87 0.53118
78 -> 88 0.15041
79 -> 87 -0.17517
79 -> 88 0.32870

Excited State 27: Singlet-A 5.9389 eV 208.77 nm f=0.0885 <S**2>=0.000
70 -> 80 0.10867

72 -> 80 -0.29832
75 -> 81 -0.12102
77 -> 83 -0.36236
77 -> 84 0.37219
78 -> 83 0.10252
79 -> 89 -0.16071
79 -> 91 0.11536

Excited State 28: Singlet-A 5.9513 eV 208.33 nm f=0.1617 <S**2>=0.000
72 -> 80 0.59131
77 -> 83 -0.14268
77 -> 84 0.13861
79 -> 89 -0.19012

Excited State 29: Singlet-A 5.9672 eV 207.78 nm f=0.0139 <S**2>=0.000
72 -> 80 0.12170
77 -> 83 -0.19337
77 -> 84 0.16130
78 -> 87 -0.13769
78 -> 89 0.15312
79 -> 88 0.26648
79 -> 89 0.52795

Excited State 30: Singlet-A 6.0179 eV 206.02 nm f=0.2351 <S**2>=0.000
75 -> 81 0.53476
77 -> 83 -0.24989
78 -> 83 -0.13950
79 -> 88 -0.12705
79 -> 91 -0.16459

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8526 eV 434.64 nm f=0.5908 <S**2>=0.000
79 -> 80 0.70360
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.59496270
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1229 eV 397.01 nm f=0.1451 <S**2>=0.000
78 -> 80 0.70297

Excited State 3: Singlet-A 3.7925 eV 326.92 nm f=0.0451 <S**2>=0.000
73 -> 80 0.56769
74 -> 80 0.23574
75 -> 80 -0.21924
77 -> 80 0.22417

Excited State 4: Singlet-A 3.8830 eV 319.30 nm f=0.3212 <S**2>=0.000
73 -> 80 -0.24448
77 -> 80 0.58080
79 -> 81 0.29152

Excited State 5: Singlet-A 4.0149 eV 308.81 nm f=0.0884 <S**2>=0.000
77 -> 80 -0.30009
78 -> 83 -0.16759
79 -> 81 0.58293
79 -> 83 -0.11324

Excited State 6: Singlet-A 4.0322 eV 307.48 nm f=0.0112 <S**2>=0.000
76 -> 80 0.68352
79 -> 82 -0.12620

Excited State 7: Singlet-A 4.2583 eV 291.16 nm f=0.0492 <S**2>=0.000
78 -> 81 0.63299
79 -> 81 0.16799
79 -> 83 0.22468

Excited State 8: Singlet-A 4.4629 eV 277.81 nm f=0.0006 <S**2>=0.000
70 -> 80 0.66857
72 -> 80 0.17789

Excited State 9: Singlet-A 4.6063 eV 269.16 nm f=0.0407 <S**2>=0.000
73 -> 80 0.22036
74 -> 80 -0.16124
75 -> 80 0.49384
79 -> 82 0.33334
79 -> 83 0.12892

Excited State 10: Singlet-A 4.6295 eV 267.81 nm f=0.0071 <S**2>=0.000
73 -> 80 -0.14176
74 -> 80 0.10595
75 -> 80 -0.31871
76 -> 80 0.11523
78 -> 82 -0.14030
79 -> 82 0.55763

Excited State 11: Singlet-A 4.7606 eV 260.44 nm f=0.4348 <S**2>=0.000
77 -> 81 -0.35155
78 -> 81 -0.21492
78 -> 83 0.15396
78 -> 84 -0.14778
79 -> 81 0.10923
79 -> 82 -0.12154
79 -> 83 0.46774

Excited State 12: Singlet-A 4.9455 eV 250.70 nm f=0.0010 <S**2>=0.000
73 -> 80 -0.13956
74 -> 80 0.60109
75 -> 80 0.27240
78 -> 83 -0.10190

Excited State 13: Singlet-A 4.9797 eV 248.98 nm f=0.0949 <S**2>=0.000
74 -> 80 -0.11280
77 -> 81 0.41968
78 -> 83 -0.25120
79 -> 83 0.36891
79 -> 84 0.29849

Excited State 14: Singlet-A 5.0305 eV 246.46 nm f=0.0041 <S**2>=0.000
78 -> 82 0.66447
79 -> 82 0.18453
79 -> 84 0.10134

Excited State 15: Singlet-A 5.1537 eV 240.57 nm f=0.0754 <S**2>=0.000
78 -> 82 -0.10998
78 -> 83 0.37181

79 -> 83 -0.15592
79 -> 84 0.52782

Excited State 16: Singlet-A 5.2625 eV 235.60 nm f=0.0058 <S**2>=0.000
79 -> 85 0.67921
79 -> 88 0.11464

Excited State 17: Singlet-A 5.3497 eV 231.76 nm f=0.0707 <S**2>=0.000
74 -> 81 0.10613
75 -> 81 0.12293
78 -> 84 0.46366
78 -> 86 0.14686
79 -> 83 0.10562
79 -> 86 0.44887

Excited State 18: Singlet-A 5.3625 eV 231.21 nm f=0.0160 <S**2>=0.000
78 -> 83 0.17053
78 -> 84 0.46706
79 -> 86 -0.45622

Excited State 19: Singlet-A 5.4714 eV 226.60 nm f=0.4518 <S**2>=0.000
72 -> 80 -0.29484
75 -> 81 -0.24163
77 -> 81 0.33114
78 -> 83 0.32736
78 -> 86 -0.13639
79 -> 84 -0.21782

Excited State 20: Singlet-A 5.5093 eV 225.04 nm f=0.0521 <S**2>=0.000
70 -> 80 -0.15901
72 -> 80 0.57229
75 -> 81 -0.15673
78 -> 86 -0.14287
79 -> 84 -0.10203
79 -> 86 0.10463

Excited State 21: Singlet-A 5.5489 eV 223.44 nm f=0.0030 <S**2>=0.000
78 -> 85 0.56982
78 -> 86 0.10065
78 -> 87 0.16280
79 -> 87 0.31217

Excited State 22: Singlet-A 5.5687 eV 222.65 nm f=0.0155 <S**2>=0.000
76 -> 81 0.50714
76 -> 84 0.12239
77 -> 82 -0.39129
78 -> 86 -0.14891

Excited State 23: Singlet-A 5.6103 eV 221.00 nm f=0.2203 <S**2>=0.000
74 -> 81 0.21860
76 -> 81 0.11854
77 -> 81 0.11892
78 -> 83 0.12013
78 -> 84 -0.10058
78 -> 86 0.55735
79 -> 84 -0.12380
79 -> 86 -0.14168

Excited State 24: Singlet-A 5.7190 eV 216.79 nm f=0.0061 <S**2>=0.000

71 -> 80 0.16941
76 -> 81 0.41569
77 -> 82 0.44180
78 -> 85 -0.11893
79 -> 87 0.19943

Excited State 25: Singlet-A 5.7253 eV 216.56 nm f=0.0015 <S**2>=0.000
76 -> 81 -0.15309
77 -> 82 -0.17648
78 -> 85 -0.30480
78 -> 88 -0.10758
79 -> 87 0.50699
79 -> 88 -0.22267

Excited State 26: Singlet-A 5.7896 eV 214.15 nm f=0.0016 <S**2>=0.000
78 -> 87 -0.21462
79 -> 85 -0.10303
79 -> 87 0.23408
79 -> 88 0.58726
79 -> 89 -0.12270

Excited State 27: Singlet-A 5.9161 eV 209.57 nm f=0.0886 <S**2>=0.000
71 -> 80 0.65605
77 -> 82 -0.13146

Excited State 28: Singlet-A 5.9276 eV 209.17 nm f=0.0594 <S**2>=0.000
75 -> 81 -0.17867
78 -> 87 0.44567
78 -> 88 -0.18799
78 -> 89 -0.11734
79 -> 88 0.11661
79 -> 89 -0.37648

Excited State 29: Singlet-A 5.9616 eV 207.97 nm f=0.3913 <S**2>=0.000
75 -> 81 0.41188
77 -> 81 0.14697
77 -> 83 -0.27941
77 -> 84 -0.17440
78 -> 83 0.19741
78 -> 87 0.15757
79 -> 84 -0.12768
79 -> 89 -0.14188

Excited State 30: Singlet-A 6.0066 eV 206.41 nm f=0.0014 <S**2>=0.000
78 -> 87 0.17800
78 -> 88 -0.41006
79 -> 88 0.18446
79 -> 89 0.45565

Single-point TDDFT B3LYP/jul-cc-pV(T+d)Z/PCM(DMSO) over B3LYP/6-311++G(2df,2p)/PCM(DMSO) geometry

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7468 eV 451.38 nm f=0.2146 <S**2>=0.000

79 -> 80 0.70588
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.60372281
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1496 eV 393.65 nm f=0.4537 <S**2>=0.000
78 -> 80 0.70307

Excited State 3: Singlet-A 3.8259 eV 324.06 nm f=0.0000 <S**2>=0.000
73 -> 80 0.18591
74 -> 80 0.66996

Excited State 4: Singlet-A 3.9796 eV 311.55 nm f=0.3338 <S**2>=0.000
77 -> 80 -0.41731
79 -> 81 0.54815

Excited State 5: Singlet-A 4.0736 eV 304.36 nm f=0.1284 <S**2>=0.000
76 -> 80 0.10505
77 -> 80 0.54764
79 -> 81 0.39980
79 -> 83 0.10209

Excited State 6: Singlet-A 4.1411 eV 299.40 nm f=0.0076 <S**2>=0.000
76 -> 80 0.65543
78 -> 82 -0.11974
79 -> 82 -0.14073

Excited State 7: Singlet-A 4.1959 eV 295.49 nm f=0.0420 <S**2>=0.000
78 -> 81 0.58929
79 -> 81 -0.10802
79 -> 82 0.10694
79 -> 83 0.31337
79 -> 84 -0.12307

Excited State 8: Singlet-A 4.4558 eV 278.25 nm f=0.0004 <S**2>=0.000
70 -> 80 0.67017
73 -> 80 0.18045

Excited State 9: Singlet-A 4.4868 eV 276.33 nm f=0.0484 <S**2>=0.000
76 -> 80 0.16913
78 -> 81 -0.10540
78 -> 82 0.11932
79 -> 82 0.66145

Excited State 10: Singlet-A 4.7245 eV 262.43 nm f=0.0040 <S**2>=0.000
75 -> 80 0.69176

Excited State 11: Singlet-A 4.8301 eV 256.69 nm f=0.6244 <S**2>=0.000
77 -> 81 -0.22887
78 -> 81 -0.29719
78 -> 82 0.21622
78 -> 84 0.11873
79 -> 83 0.51884

Excited State 12: Singlet-A 4.8976 eV 253.15 nm f=0.2231 <S**2>=0.000
78 -> 81 0.10629
78 -> 82 0.63390
79 -> 82 -0.13235
79 -> 83 -0.17302

Excited State 13: Singlet-A 4.9956 eV 248.18 nm f=0.0002 <S**2>=0.000
70 -> 80 -0.18300
73 -> 80 0.64906
74 -> 80 -0.18168

Excited State 14: Singlet-A 5.1330 eV 241.54 nm f=0.0015 <S**2>=0.000
75 -> 81 -0.11244
77 -> 81 0.36831
79 -> 83 0.17795
79 -> 84 0.52607
79 -> 86 -0.13995

Excited State 15: Singlet-A 5.2690 eV 235.31 nm f=0.0001 <S**2>=0.000
79 -> 85 0.65649
79 -> 87 0.22504

Excited State 16: Singlet-A 5.2839 eV 234.65 nm f=0.0627 <S**2>=0.000
75 -> 81 0.12093
77 -> 81 0.30606
78 -> 83 0.50600
79 -> 83 0.10654
79 -> 84 -0.20316
79 -> 86 0.24964

Excited State 17: Singlet-A 5.3676 eV 230.99 nm f=0.0035 <S**2>=0.000
72 -> 80 -0.16357
75 -> 81 0.19191
78 -> 83 -0.23777
79 -> 84 0.21269
79 -> 86 0.56127

Excited State 18: Singlet-A 5.4636 eV 226.93 nm f=0.0166 <S**2>=0.000
72 -> 80 0.66714
77 -> 81 0.10127
78 -> 83 -0.10355
79 -> 86 0.13517

Excited State 19: Singlet-A 5.5504 eV 223.38 nm f=0.0003 <S**2>=0.000
78 -> 85 -0.33080
79 -> 85 -0.15177
79 -> 87 0.53525
79 -> 88 -0.24207

Excited State 20: Singlet-A 5.5877 eV 221.89 nm f=0.0350 <S**2>=0.000
75 -> 83 0.11596
78 -> 84 0.62694
78 -> 86 -0.20100

Excited State 21: Singlet-A 5.6441 eV 219.67 nm f=0.2115 <S**2>=0.000
76 -> 81 0.22496
76 -> 84 -0.12303
77 -> 81 -0.20162
77 -> 82 0.50883
78 -> 83 0.20896
79 -> 84 0.14188

Excited State 22: Singlet-A 5.7059 eV 217.29 nm f=0.0005 <S**2>=0.000
78 -> 85 0.58450

79 -> 85 -0.10973
79 -> 87 0.23595
79 -> 88 -0.23284

Excited State 23: Singlet-A 5.7285 eV 216.43 nm f=0.5058 <S**2>=0.000
76 -> 81 0.37602
77 -> 81 0.33518
77 -> 82 0.18975
78 -> 83 -0.28063
79 -> 83 0.12986
79 -> 84 -0.23355
79 -> 86 -0.10589

Excited State 24: Singlet-A 5.7938 eV 214.00 nm f=0.1524 <S**2>=0.000
75 -> 81 -0.24176
75 -> 83 -0.12065
78 -> 83 -0.10034
78 -> 84 0.22102
78 -> 86 0.54546
79 -> 84 -0.11251
79 -> 86 0.11767

Excited State 25: Singlet-A 5.8078 eV 213.48 nm f=0.0012 <S**2>=0.000
79 -> 87 0.21584
79 -> 88 0.48687
79 -> 89 -0.40423
79 -> 90 0.16279

Excited State 26: Singlet-A 5.8726 eV 211.12 nm f=0.0626 <S**2>=0.000
71 -> 80 0.34565
76 -> 81 0.47349
77 -> 81 -0.11006
77 -> 82 -0.27448
78 -> 83 0.10680
78 -> 86 0.14466
79 -> 84 0.10419

Excited State 27: Singlet-A 5.8951 eV 210.32 nm f=0.0004 <S**2>=0.000
78 -> 87 0.30382
79 -> 85 -0.11199
79 -> 87 0.19273
79 -> 88 0.26595
79 -> 89 0.49605
79 -> 92 0.14404

Excited State 28: Singlet-A 5.9579 eV 208.10 nm f=0.0244 <S**2>=0.000
71 -> 80 -0.30369
75 -> 81 0.51624
78 -> 86 0.25590
79 -> 86 -0.17243

Excited State 29: Singlet-A 5.9818 eV 207.27 nm f=0.0000 <S**2>=0.000
73 -> 81 0.64952
74 -> 81 -0.22089

Excited State 30: Singlet-A 5.9835 eV 207.21 nm f=0.0487 <S**2>=0.000
71 -> 80 0.50279
75 -> 81 0.28656
76 -> 81 -0.24349

77 -> 82 0.23894

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4769 eV 500.57 nm f=0.9450 <S**2>=0.000
79 -> 80 0.70422
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.14571407
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9952 eV 413.94 nm f=0.2088 <S**2>=0.000
78 -> 80 0.69855

Excited State 3: Singlet-A 3.5887 eV 345.48 nm f=0.2625 <S**2>=0.000
77 -> 80 0.24036
79 -> 81 0.64929

Excited State 4: Singlet-A 3.7409 eV 331.43 nm f=0.0000 <S**2>=0.000
72 -> 80 0.57885
73 -> 80 0.18067
76 -> 80 -0.34171

Excited State 5: Singlet-A 3.8635 eV 320.91 nm f=0.0699 <S**2>=0.000
77 -> 80 0.63574
78 -> 83 -0.10526
79 -> 81 -0.20526
79 -> 83 0.15781

Excited State 6: Singlet-A 3.9946 eV 310.38 nm f=0.0001 <S**2>=0.000
72 -> 80 0.32747
76 -> 80 0.61217

Excited State 7: Singlet-A 4.0050 eV 309.58 nm f=0.0050 <S**2>=0.000
75 -> 80 0.53707
79 -> 82 -0.43810

Excited State 8: Singlet-A 4.1141 eV 301.36 nm f=0.0039 <S**2>=0.000
75 -> 80 -0.34457
78 -> 81 0.42160
79 -> 82 -0.38327
79 -> 83 -0.17438

Excited State 9: Singlet-A 4.1721 eV 297.18 nm f=0.0671 <S**2>=0.000
75 -> 80 0.27850
78 -> 81 0.42697
79 -> 82 0.37653
79 -> 83 -0.28238

Excited State 10: Singlet-A 4.4781 eV 276.87 nm f=0.0001 <S**2>=0.000
69 -> 80 0.52853
72 -> 80 0.13583
73 -> 80 -0.43428

Excited State 11: Singlet-A 4.4905 eV 276.10 nm f=0.4032 <S**2>=0.000
77 -> 80 -0.12621
77 -> 81 0.11186
78 -> 81 0.32759

79 -> 83 0.56650
79 -> 85 0.12696

Excited State 12: Singlet-A 4.6056 eV 269.20 nm f=0.0008 <S**2>=0.000
69 -> 80 0.44899
72 -> 80 -0.14523
73 -> 80 0.51205

Excited State 13: Singlet-A 4.6430 eV 267.04 nm f=0.0003 <S**2>=0.000
79 -> 84 0.68769
79 -> 88 0.10166

Excited State 14: Singlet-A 4.7030 eV 263.63 nm f=0.0110 <S**2>=0.000
74 -> 80 0.59665
77 -> 81 -0.10314
79 -> 85 0.33437

Excited State 15: Singlet-A 4.7853 eV 259.10 nm f=0.0341 <S**2>=0.000
74 -> 80 0.11580
77 -> 81 0.46609
78 -> 82 -0.26904
78 -> 83 -0.37032
79 -> 83 -0.15811

Excited State 16: Singlet-A 4.8529 eV 255.48 nm f=0.0244 <S**2>=0.000
74 -> 80 -0.34302
78 -> 81 -0.10182
79 -> 85 0.56513
79 -> 87 -0.12568

Excited State 17: Singlet-A 4.9433 eV 250.81 nm f=0.0053 <S**2>=0.000
78 -> 84 -0.14036
79 -> 86 0.67802

Excited State 18: Singlet-A 4.9866 eV 248.63 nm f=0.0611 <S**2>=0.000
77 -> 81 0.13323
78 -> 82 0.62449
78 -> 83 -0.22827
79 -> 87 -0.13768

Excited State 19: Singlet-A 5.0329 eV 246.35 nm f=0.0500 <S**2>=0.000
71 -> 80 -0.15692
78 -> 83 -0.18357
79 -> 87 0.62988

Excited State 20: Singlet-A 5.1511 eV 240.69 nm f=0.0011 <S**2>=0.000
78 -> 84 0.14444
78 -> 86 0.12011
79 -> 88 0.65759
79 -> 89 -0.10257

Excited State 21: Singlet-A 5.2459 eV 236.34 nm f=0.0001 <S**2>=0.000
79 -> 88 0.10178
79 -> 89 0.66840

Excited State 22: Singlet-A 5.2475 eV 236.27 nm f=0.0508 <S**2>=0.000
71 -> 80 0.62624
77 -> 81 -0.15968
78 -> 83 -0.15830

78 -> 85 -0.14187
79 -> 87 0.13312

Excited State 23: Singlet-A 5.2865 eV 234.53 nm f=0.0007 <S**2>=0.000
78 -> 84 0.60367
78 -> 86 0.25696
79 -> 86 0.12946
79 -> 88 -0.16785

Excited State 24: Singlet-A 5.3301 eV 232.61 nm f=0.0104 <S**2>=0.000
71 -> 80 0.19872
74 -> 81 -0.15940
78 -> 83 0.13280
78 -> 85 0.60452
78 -> 87 -0.17414

Excited State 25: Singlet-A 5.3827 eV 230.34 nm f=0.0002 <S**2>=0.000
76 -> 81 0.68575

Excited State 26: Singlet-A 5.4800 eV 226.25 nm f=0.0000 <S**2>=0.000
78 -> 88 0.14047
79 -> 89 0.10191
79 -> 90 0.66488

Excited State 27: Singlet-A 5.5510 eV 223.35 nm f=0.7722 <S**2>=0.000
71 -> 80 0.14449
74 -> 81 0.13175
77 -> 81 0.39765
77 -> 82 0.20049
78 -> 83 0.40316
78 -> 87 0.11216
79 -> 85 0.12599
79 -> 87 0.15970

Excited State 28: Singlet-A 5.6020 eV 221.32 nm f=0.0004 <S**2>=0.000
78 -> 84 -0.18419
78 -> 86 0.51113
78 -> 88 -0.28901
78 -> 89 -0.18313
79 -> 90 0.14392
79 -> 91 0.20100

Excited State 29: Singlet-A 5.6290 eV 220.26 nm f=0.0094 <S**2>=0.000
75 -> 81 0.52253
77 -> 82 -0.41027
78 -> 87 0.10046

Excited State 30: Singlet-A 5.6697 eV 218.68 nm f=0.0003 <S**2>=0.000
72 -> 81 -0.12289
73 -> 81 0.67387

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7053 eV 458.30 nm f=0.3570 <S**2>=0.000
79 -> 80 0.70629
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.60277803

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

Excited State 2: Singlet-A 3.1639 eV 391.88 nm f=0.3631 <S**2>=0.000
78 -> 80 0.70257

Excited State 3: Singlet-A 3.8232 eV 324.29 nm f=0.0000 <S**2>=0.000
74 -> 80 0.69460

Excited State 4: Singlet-A 3.9214 eV 316.17 nm f=0.3638 <S**2>=0.000
77 -> 80 -0.25916
79 -> 81 0.63556

Excited State 5: Singlet-A 4.0463 eV 306.42 nm f=0.0825 <S**2>=0.000
77 -> 80 0.63994
79 -> 81 0.24056
79 -> 83 0.10909

Excited State 6: Singlet-A 4.1516 eV 298.64 nm f=0.0069 <S**2>=0.000
76 -> 80 0.63772
78 -> 82 -0.12305
79 -> 82 -0.22621

Excited State 7: Singlet-A 4.2161 eV 294.07 nm f=0.0263 <S**2>=0.000
78 -> 81 0.58078
79 -> 81 -0.10802
79 -> 83 0.33265
79 -> 84 -0.13414

Excited State 8: Singlet-A 4.4144 eV 280.86 nm f=0.0178 <S**2>=0.000
76 -> 80 0.24571
79 -> 82 0.65124

Excited State 9: Singlet-A 4.4625 eV 277.84 nm f=0.0005 <S**2>=0.000
70 -> 80 0.69454

Excited State 10: Singlet-A 4.7396 eV 261.59 nm f=0.0025 <S**2>=0.000
75 -> 80 0.69648

Excited State 11: Singlet-A 4.7718 eV 259.83 nm f=0.6954 <S**2>=0.000
77 -> 81 -0.20987
78 -> 81 -0.34029
78 -> 82 0.16245
78 -> 84 0.10845
79 -> 83 0.52411

Excited State 12: Singlet-A 4.9001 eV 253.03 nm f=0.0870 <S**2>=0.000
78 -> 82 0.65002
79 -> 82 -0.10464
79 -> 83 -0.16904
79 -> 84 -0.11309

Excited State 13: Singlet-A 5.0797 eV 244.08 nm f=0.0025 <S**2>=0.000
77 -> 81 0.41355
78 -> 82 0.11201
79 -> 83 0.16716
79 -> 84 0.48447
79 -> 86 -0.11481

Excited State 14: Singlet-A 5.1461 eV 240.93 nm f=0.0002 <S**2>=0.000

73 -> 80 0.69701

Excited State 15: Singlet-A 5.1814 eV 239.29 nm f=0.0004 <S**2>=0.000
79 -> 85 0.66800
79 -> 87 0.16893

Excited State 16: Singlet-A 5.2512 eV 236.11 nm f=0.0387 <S**2>=0.000
75 -> 81 0.11815
77 -> 81 0.28878
78 -> 83 0.46944
79 -> 83 0.10132
79 -> 84 -0.24287
79 -> 86 0.30642

Excited State 17: Singlet-A 5.3356 eV 232.37 nm f=0.0171 <S**2>=0.000
72 -> 80 -0.13939
75 -> 81 0.16308
78 -> 83 -0.26607
79 -> 84 0.22542
79 -> 86 0.55773

Excited State 18: Singlet-A 5.4684 eV 226.73 nm f=0.0154 <S**2>=0.000
72 -> 80 0.67086
78 -> 83 -0.11889
79 -> 86 0.11192

Excited State 19: Singlet-A 5.4936 eV 225.69 nm f=0.0010 <S**2>=0.000
78 -> 85 -0.24010
79 -> 85 -0.10829
79 -> 87 0.60801
79 -> 88 -0.19245

Excited State 20: Singlet-A 5.5994 eV 221.42 nm f=0.0447 <S**2>=0.000
75 -> 83 0.12031
77 -> 83 -0.13303
78 -> 84 0.60015
78 -> 86 -0.20344
79 -> 84 0.12790

Excited State 21: Singlet-A 5.6311 eV 220.18 nm f=0.1965 <S**2>=0.000
76 -> 81 0.22343
76 -> 83 -0.10367
76 -> 84 -0.11238
77 -> 81 -0.19293
77 -> 82 0.52373
78 -> 83 0.19053
79 -> 84 0.15359

Excited State 22: Singlet-A 5.7204 eV 216.74 nm f=0.0006 <S**2>=0.000
78 -> 85 0.62298
79 -> 87 0.21507
79 -> 89 -0.14345

Excited State 23: Singlet-A 5.7408 eV 215.97 nm f=0.6084 <S**2>=0.000
76 -> 81 0.33750
77 -> 81 0.33602
77 -> 82 0.18794
78 -> 83 -0.31451
78 -> 84 0.10346

78 -> 86 -0.11614
79 -> 84 -0.23397

Excited State 24: Singlet-A 5.7617 eV 215.19 nm f=0.0000 <S**2>=0.000
79 -> 85 -0.10220
79 -> 87 0.10518
79 -> 88 0.58150
79 -> 89 -0.27858
79 -> 90 0.21279

Excited State 25: Singlet-A 5.8069 eV 213.51 nm f=0.1099 <S**2>=0.000
75 -> 81 -0.33281
78 -> 84 0.24217
78 -> 86 0.50187
79 -> 86 0.14555

Excited State 26: Singlet-A 5.8725 eV 211.13 nm f=0.0010 <S**2>=0.000
78 -> 87 0.23630
79 -> 87 0.15389
79 -> 88 0.20532
79 -> 89 0.57452
79 -> 92 -0.14721

Excited State 27: Singlet-A 5.8753 eV 211.03 nm f=0.1011 <S**2>=0.000
71 -> 80 0.40076
76 -> 81 0.46756
77 -> 81 -0.11415
77 -> 82 -0.23274
78 -> 83 0.12145

Excited State 28: Singlet-A 5.9692 eV 207.71 nm f=0.0614 <S**2>=0.000
71 -> 80 0.54665
76 -> 81 -0.30465
77 -> 82 0.25377

Excited State 29: Singlet-A 5.9917 eV 206.93 nm f=0.0051 <S**2>=0.000
75 -> 81 0.55175
78 -> 86 0.35984
79 -> 86 -0.14375

Excited State 30: Singlet-A 5.9938 eV 206.85 nm f=0.0000 <S**2>=0.000
78 -> 87 0.29651
78 -> 88 -0.22405
79 -> 88 -0.21227
79 -> 90 0.52929

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4527 eV 505.50 nm f=0.9932 <S**2>=0.000
79 -> 80 0.70445
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.14373970
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0227 eV 410.18 nm f=0.1388 <S**2>=0.000
78 -> 80 0.69456
79 -> 81 0.11485

Excited State 3: Singlet-A 3.5103 eV 353.20 nm f=0.2758 <S**2>=0.000
77 -> 80 0.36736
79 -> 81 0.58315

Excited State 4: Singlet-A 3.6988 eV 335.20 nm f=0.0293 <S**2>=0.000
72 -> 80 0.27487
74 -> 80 -0.11724
75 -> 80 -0.10087
76 -> 80 0.20171
77 -> 80 0.46746
79 -> 81 -0.32407
79 -> 83 -0.10702

Excited State 5: Singlet-A 3.7805 eV 327.95 nm f=0.0149 <S**2>=0.000
72 -> 80 0.57056
74 -> 80 -0.13295
76 -> 80 0.10675
77 -> 80 -0.31350
79 -> 81 0.12644

Excited State 6: Singlet-A 3.9913 eV 310.64 nm f=0.0007 <S**2>=0.000
75 -> 80 -0.30834
76 -> 80 -0.18919
79 -> 82 0.59585

Excited State 7: Singlet-A 4.1042 eV 302.09 nm f=0.0238 <S**2>=0.000
72 -> 80 -0.12592
75 -> 80 0.15679
76 -> 80 0.41482
78 -> 81 0.30559
79 -> 82 0.21521
79 -> 83 0.35318

Excited State 8: Singlet-A 4.1388 eV 299.57 nm f=0.0197 <S**2>=0.000
75 -> 80 0.45703
76 -> 80 0.16206
78 -> 81 -0.31617
79 -> 82 0.28604
79 -> 83 -0.25451

Excited State 9: Singlet-A 4.1977 eV 295.36 nm f=0.0032 <S**2>=0.000
72 -> 80 -0.19798
75 -> 80 -0.37365
76 -> 80 0.40943
77 -> 80 -0.14338
78 -> 81 -0.31978

Excited State 10: Singlet-A 4.4357 eV 279.51 nm f=0.3918 <S**2>=0.000
76 -> 80 -0.12476
77 -> 80 0.12559
77 -> 81 -0.10331
78 -> 81 -0.40270
79 -> 83 0.49183
79 -> 84 0.13834
79 -> 85 -0.11630

Excited State 11: Singlet-A 4.5229 eV 274.13 nm f=0.0007 <S**2>=0.000
69 -> 80 0.69215

Excited State 12: Singlet-A 4.5779 eV 270.83 nm f=0.0085 <S**2>=0.000
79 -> 84 0.63550
79 -> 85 0.24166
79 -> 88 0.13631

Excited State 13: Singlet-A 4.6942 eV 264.12 nm f=0.0128 <S**2>=0.000
73 -> 80 0.34435
74 -> 80 0.28432
77 -> 81 -0.30102
78 -> 81 -0.10166
78 -> 83 -0.12135
79 -> 85 0.38768

Excited State 14: Singlet-A 4.7042 eV 263.56 nm f=0.0036 <S**2>=0.000
73 -> 80 0.60658
74 -> 80 -0.18016
77 -> 81 0.15904
79 -> 85 -0.20136

Excited State 15: Singlet-A 4.7553 eV 260.73 nm f=0.0116 <S**2>=0.000
74 -> 80 0.28113
77 -> 81 0.42666
78 -> 83 0.32986
79 -> 83 0.15105
79 -> 85 0.17727
79 -> 87 0.18396

Excited State 16: Singlet-A 4.8589 eV 255.17 nm f=0.0083 <S**2>=0.000
74 -> 80 0.50143
79 -> 84 0.13536
79 -> 85 -0.35937
79 -> 87 -0.22147

Excited State 17: Singlet-A 4.8900 eV 253.55 nm f=0.0046 <S**2>=0.000
78 -> 84 -0.12298
79 -> 86 0.67701

Excited State 18: Singlet-A 4.9598 eV 249.98 nm f=0.0281 <S**2>=0.000
78 -> 82 0.58042
79 -> 87 -0.36059

Excited State 19: Singlet-A 4.9808 eV 248.93 nm f=0.0532 <S**2>=0.000
71 -> 80 -0.10573
78 -> 82 0.36123
78 -> 83 -0.21942
79 -> 85 -0.17560
79 -> 87 0.48543

Excited State 20: Singlet-A 5.1232 eV 242.00 nm f=0.0024 <S**2>=0.000
79 -> 84 -0.12523
79 -> 88 0.66357
79 -> 89 0.12340

Excited State 21: Singlet-A 5.2100 eV 237.97 nm f=0.0089 <S**2>=0.000
78 -> 86 -0.10530
79 -> 88 -0.11132
79 -> 89 0.67039

Excited State 22: Singlet-A 5.2356 eV 236.81 nm f=0.3583 <S**2>=0.000
71 -> 80 0.38341
75 -> 81 -0.13540
76 -> 81 0.28506
77 -> 81 0.30348
78 -> 83 -0.33916

Excited State 23: Singlet-A 5.3184 eV 233.12 nm f=0.0015 <S**2>=0.000
78 -> 84 0.60694
78 -> 85 0.13029
78 -> 86 0.22051
79 -> 86 0.12939

Excited State 24: Singlet-A 5.3390 eV 232.22 nm f=0.0478 <S**2>=0.000
71 -> 80 0.40856
75 -> 81 0.11117
76 -> 81 -0.30296
77 -> 81 -0.10404
77 -> 82 0.12969
78 -> 85 0.34305
78 -> 87 0.12131
79 -> 87 0.14909

Excited State 25: Singlet-A 5.3611 eV 231.26 nm f=0.0172 <S**2>=0.000
71 -> 80 -0.35710
74 -> 81 -0.13161
78 -> 83 -0.20041
78 -> 85 0.49835
78 -> 87 0.12294

Excited State 26: Singlet-A 5.4223 eV 228.65 nm f=0.0007 <S**2>=0.000
79 -> 90 0.67789

Excited State 27: Singlet-A 5.4690 eV 226.71 nm f=0.0046 <S**2>=0.000
75 -> 81 -0.21662
76 -> 82 0.16374
77 -> 82 0.60850

Excited State 28: Singlet-A 5.6024 eV 221.31 nm f=0.0092 <S**2>=0.000
78 -> 84 -0.12027
78 -> 86 0.48522
78 -> 87 -0.11447
78 -> 88 -0.23660
78 -> 89 0.11117
79 -> 91 0.33604

Excited State 29: Singlet-A 5.6503 eV 219.43 nm f=0.0648 <S**2>=0.000
74 -> 81 -0.14147
76 -> 81 0.22886
78 -> 83 0.19466
78 -> 87 0.52669
79 -> 91 0.23951

Excited State 30: Singlet-A 5.6798 eV 218.29 nm f=0.0125 <S**2>=0.000
78 -> 84 0.16344
78 -> 86 -0.34281
78 -> 87 -0.14074
79 -> 91 0.52865

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8626 eV 433.12 nm f=0.3315 <S**2>=0.000
79 -> 80 0.69853
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.59305938
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1067 eV 399.09 nm f=0.1722 <S**2>=0.000
78 -> 80 0.69879

Excited State 3: Singlet-A 3.7888 eV 327.24 nm f=0.2665 <S**2>=0.000
73 -> 80 0.39180
74 -> 80 0.13871
75 -> 80 0.14014
77 -> 80 0.52414
79 -> 81 -0.13347

Excited State 4: Singlet-A 3.8368 eV 323.15 nm f=0.1437 <S**2>=0.000
73 -> 80 0.52376
74 -> 80 0.12132
77 -> 80 -0.41930
79 -> 81 0.10982

Excited State 5: Singlet-A 4.0683 eV 304.75 nm f=0.1431 <S**2>=0.000
76 -> 80 -0.23157
77 -> 80 0.15414
78 -> 81 -0.18487
78 -> 83 -0.17272
79 -> 81 0.56764
79 -> 83 -0.13554

Excited State 6: Singlet-A 4.0923 eV 302.97 nm f=0.0384 <S**2>=0.000
76 -> 80 0.63729
79 -> 81 0.19200
79 -> 82 -0.12143

Excited State 7: Singlet-A 4.2534 eV 291.49 nm f=0.0548 <S**2>=0.000
78 -> 81 0.60826
79 -> 81 0.25884
79 -> 83 0.21918

Excited State 8: Singlet-A 4.4660 eV 277.62 nm f=0.0005 <S**2>=0.000
71 -> 80 0.69101

Excited State 9: Singlet-A 4.5689 eV 271.36 nm f=0.0114 <S**2>=0.000
76 -> 80 0.15019
78 -> 82 -0.21334
79 -> 82 0.64414

Excited State 10: Singlet-A 4.6702 eV 265.48 nm f=0.0302 <S**2>=0.000
73 -> 80 -0.19525
74 -> 80 0.20865
75 -> 80 0.60706
79 -> 83 0.10304

Excited State 11: Singlet-A 4.8063 eV 257.96 nm f=0.3854 <S**2>=0.000

75 -> 80 0.11680
77 -> 81 0.44540
78 -> 81 0.21127
78 -> 83 -0.16582
78 -> 84 -0.13766
79 -> 81 -0.10914
79 -> 83 -0.38945

Excited State 12: Singlet-A 4.9191 eV 252.05 nm f=0.0025 <S**2>=0.000
74 -> 80 0.11368
78 -> 82 0.64631
79 -> 82 0.22948

Excited State 13: Singlet-A 4.9355 eV 251.21 nm f=0.0025 <S**2>=0.000
73 -> 80 -0.10899
74 -> 80 0.62188
75 -> 80 -0.26119
78 -> 82 -0.12089

Excited State 14: Singlet-A 5.0446 eV 245.78 nm f=0.2320 <S**2>=0.000
77 -> 81 -0.38156
78 -> 83 0.16294
79 -> 83 -0.34892
79 -> 84 0.42434

Excited State 15: Singlet-A 5.1848 eV 239.13 nm f=0.0528 <S**2>=0.000
78 -> 81 -0.10656
78 -> 83 -0.39644
79 -> 83 0.29372
79 -> 84 0.45822

Excited State 16: Singlet-A 5.3320 eV 232.53 nm f=0.0034 <S**2>=0.000
78 -> 84 0.10913
79 -> 85 0.66962
79 -> 87 -0.10223

Excited State 17: Singlet-A 5.3469 eV 231.88 nm f=0.1150 <S**2>=0.000
75 -> 81 0.10104
77 -> 81 0.10819
78 -> 84 0.62265
78 -> 86 -0.10360
79 -> 83 -0.11081
79 -> 84 0.11949
79 -> 85 -0.10077
79 -> 86 -0.14955

Excited State 18: Singlet-A 5.3888 eV 230.08 nm f=0.0671 <S**2>=0.000
74 -> 81 0.16622
77 -> 81 0.10901
78 -> 84 0.14276
78 -> 86 0.11136
79 -> 84 0.12892
79 -> 86 0.61702

Excited State 19: Singlet-A 5.4285 eV 228.39 nm f=0.5593 <S**2>=0.000
75 -> 81 0.26047
77 -> 81 0.30529
78 -> 83 0.42174
78 -> 84 -0.16677

78 -> 86 -0.15734
79 -> 81 0.10570
79 -> 83 0.13652
79 -> 84 0.18596

Excited State 20: Singlet-A 5.4517 eV 227.42 nm f=0.0146 <S**2>=0.000
76 -> 81 0.16172
76 -> 84 -0.16644
77 -> 82 0.63456

Excited State 21: Singlet-A 5.5629 eV 222.88 nm f=0.0036 <S**2>=0.000
78 -> 85 0.60921
78 -> 87 -0.19917
79 -> 87 -0.26060

Excited State 22: Singlet-A 5.5971 eV 221.51 nm f=0.0872 <S**2>=0.000
70 -> 80 -0.23773
74 -> 81 0.16362
78 -> 86 0.56956
79 -> 86 -0.18915

Excited State 23: Singlet-A 5.6152 eV 220.80 nm f=0.0349 <S**2>=0.000
70 -> 80 0.62877
78 -> 86 0.20912

Excited State 24: Singlet-A 5.7537 eV 215.49 nm f=0.0065 <S**2>=0.000
76 -> 81 0.31413
78 -> 85 0.23250
78 -> 88 0.12837
79 -> 87 0.51914
79 -> 88 0.16224

Excited State 25: Singlet-A 5.7548 eV 215.44 nm f=0.0154 <S**2>=0.000
76 -> 81 0.59769
77 -> 82 -0.13014
78 -> 85 -0.13002
79 -> 87 -0.27222

Excited State 26: Singlet-A 5.8994 eV 210.16 nm f=0.0032 <S**2>=0.000
77 -> 85 0.13422
78 -> 85 0.12392
78 -> 87 0.53118
78 -> 88 0.15041
79 -> 87 -0.17517
79 -> 88 0.32870

Excited State 27: Singlet-A 5.9389 eV 208.77 nm f=0.0885 <S**2>=0.000
70 -> 80 0.10867
72 -> 80 -0.29832
75 -> 81 -0.12102
77 -> 83 -0.36236
77 -> 84 0.37219
78 -> 83 0.10252
79 -> 89 -0.16071
79 -> 91 0.11536

Excited State 28: Singlet-A 5.9513 eV 208.33 nm f=0.1617 <S**2>=0.000
72 -> 80 0.59131
77 -> 83 -0.14268

77 -> 84 0.13861
79 -> 89 -0.19012

Excited State 29: Singlet-A 5.9672 eV 207.78 nm f=0.0139 <S**2>=0.000
72 -> 80 0.12170
77 -> 83 -0.19337
77 -> 84 0.16130
78 -> 87 -0.13769
78 -> 89 0.15312
79 -> 88 0.26648
79 -> 89 0.52795

Excited State 30: Singlet-A 6.0179 eV 206.02 nm f=0.2351 <S**2>=0.000
75 -> 81 0.53476
77 -> 83 -0.24989
78 -> 83 -0.13950
79 -> 88 -0.12705
79 -> 91 -0.16459

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Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8526 eV 434.64 nm f=0.5908 <S**2>=0.000
79 -> 80 0.70360
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1044.59496270
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1229 eV 397.01 nm f=0.1451 <S**2>=0.000
78 -> 80 0.70297

Excited State 3: Singlet-A 3.7925 eV 326.92 nm f=0.0451 <S**2>=0.000
73 -> 80 0.56769
74 -> 80 0.23574
75 -> 80 -0.21924
77 -> 80 0.22417

Excited State 4: Singlet-A 3.8830 eV 319.30 nm f=0.3212 <S**2>=0.000
73 -> 80 -0.24448
77 -> 80 0.58080
79 -> 81 0.29152

Excited State 5: Singlet-A 4.0149 eV 308.81 nm f=0.0884 <S**2>=0.000
77 -> 80 -0.30009
78 -> 83 -0.16759
79 -> 81 0.58293
79 -> 83 -0.11324

Excited State 6: Singlet-A 4.0322 eV 307.48 nm f=0.0112 <S**2>=0.000
76 -> 80 0.68352
79 -> 82 -0.12620

Excited State 7: Singlet-A 4.2583 eV 291.16 nm f=0.0492 <S**2>=0.000
78 -> 81 0.63299
79 -> 81 0.16799
79 -> 83 0.22468

Excited State 8: Singlet-A 4.4629 eV 277.81 nm f=0.0006 <S**2>=0.000

70 -> 80 0.66857
72 -> 80 0.17789

Excited State 9: Singlet-A 4.6063 eV 269.16 nm f=0.0407 <S**2>=0.000
73 -> 80 0.22036
74 -> 80 -0.16124
75 -> 80 0.49384
79 -> 82 0.33334
79 -> 83 0.12892

Excited State 10: Singlet-A 4.6295 eV 267.81 nm f=0.0071 <S**2>=0.000
73 -> 80 -0.14176
74 -> 80 0.10595
75 -> 80 -0.31871
76 -> 80 0.11523
78 -> 82 -0.14030
79 -> 82 0.55763

Excited State 11: Singlet-A 4.7606 eV 260.44 nm f=0.4348 <S**2>=0.000
77 -> 81 -0.35155
78 -> 81 -0.21492
78 -> 83 0.15396
78 -> 84 -0.14778
79 -> 81 0.10923
79 -> 82 -0.12154
79 -> 83 0.46774

Excited State 12: Singlet-A 4.9455 eV 250.70 nm f=0.0010 <S**2>=0.000
73 -> 80 -0.13956
74 -> 80 0.60109
75 -> 80 0.27240
78 -> 83 -0.10190

Excited State 13: Singlet-A 4.9797 eV 248.98 nm f=0.0949 <S**2>=0.000
74 -> 80 -0.11280
77 -> 81 0.41968
78 -> 83 -0.25120
79 -> 83 0.36891
79 -> 84 0.29849

Excited State 14: Singlet-A 5.0305 eV 246.46 nm f=0.0041 <S**2>=0.000
78 -> 82 0.66447
79 -> 82 0.18453
79 -> 84 0.10134

Excited State 15: Singlet-A 5.1537 eV 240.57 nm f=0.0754 <S**2>=0.000
78 -> 82 -0.10998
78 -> 83 0.37181
79 -> 83 -0.15592
79 -> 84 0.52782

Excited State 16: Singlet-A 5.2625 eV 235.60 nm f=0.0058 <S**2>=0.000
79 -> 85 0.67921
79 -> 88 0.11464

Excited State 17: Singlet-A 5.3497 eV 231.76 nm f=0.0707 <S**2>=0.000
74 -> 81 0.10613
75 -> 81 0.12293
78 -> 84 0.46366

78 -> 86 0.14686
79 -> 83 0.10562
79 -> 86 0.44887

Excited State 18: Singlet-A 5.3625 eV 231.21 nm f=0.0160 <S**2>=0.000
78 -> 83 0.17053
78 -> 84 0.46706
79 -> 86 -0.45622

Excited State 19: Singlet-A 5.4714 eV 226.60 nm f=0.4518 <S**2>=0.000
72 -> 80 -0.29484
75 -> 81 -0.24163
77 -> 81 0.33114
78 -> 83 0.32736
78 -> 86 -0.13639
79 -> 84 -0.21782

Excited State 20: Singlet-A 5.5093 eV 225.04 nm f=0.0521 <S**2>=0.000
70 -> 80 -0.15901
72 -> 80 0.57229
75 -> 81 -0.15673
78 -> 86 -0.14287
79 -> 84 -0.10203
79 -> 86 0.10463

Excited State 21: Singlet-A 5.5489 eV 223.44 nm f=0.0030 <S**2>=0.000
78 -> 85 0.56982
78 -> 86 0.10065
78 -> 87 0.16280
79 -> 87 0.31217

Excited State 22: Singlet-A 5.5687 eV 222.65 nm f=0.0155 <S**2>=0.000
76 -> 81 0.50714
76 -> 84 0.12239
77 -> 82 -0.39129
78 -> 86 -0.14891

Excited State 23: Singlet-A 5.6103 eV 221.00 nm f=0.2203 <S**2>=0.000
74 -> 81 0.21860
76 -> 81 0.11854
77 -> 81 0.11892
78 -> 83 0.12013
78 -> 84 -0.10058
78 -> 86 0.55735
79 -> 84 -0.12380
79 -> 86 -0.14168

Excited State 24: Singlet-A 5.7190 eV 216.79 nm f=0.0061 <S**2>=0.000
71 -> 80 0.16941
76 -> 81 0.41569
77 -> 82 0.44180
78 -> 85 -0.11893
79 -> 87 0.19943

Excited State 25: Singlet-A 5.7253 eV 216.56 nm f=0.0015 <S**2>=0.000
76 -> 81 -0.15309
77 -> 82 -0.17648
78 -> 85 -0.30480
78 -> 88 -0.10758

79 -> 87 0.50699
79 -> 88 -0.22267

Excited State 26: Singlet-A 5.7896 eV 214.15 nm f=0.0016 <S**2>=0.000
78 -> 87 -0.21462
79 -> 85 -0.10303
79 -> 87 0.23408
79 -> 88 0.58726
79 -> 89 -0.12270

Excited State 27: Singlet-A 5.9161 eV 209.57 nm f=0.0886 <S**2>=0.000
71 -> 80 0.65605
77 -> 82 -0.13146

Excited State 28: Singlet-A 5.9276 eV 209.17 nm f=0.0594 <S**2>=0.000
75 -> 81 -0.17867
78 -> 87 0.44567
78 -> 88 -0.18799
78 -> 89 -0.11734
79 -> 88 0.11661
79 -> 89 -0.37648

Excited State 29: Singlet-A 5.9616 eV 207.97 nm f=0.3913 <S**2>=0.000
75 -> 81 0.41188
77 -> 81 0.14697
77 -> 83 -0.27941
77 -> 84 -0.17440
78 -> 83 0.19741
78 -> 87 0.15757
79 -> 84 -0.12768
79 -> 89 -0.14188

Excited State 30: Singlet-A 6.0066 eV 206.41 nm f=0.0014 <S**2>=0.000
78 -> 87 0.17800
78 -> 88 -0.41006
79 -> 88 0.18446
79 -> 89 0.45565