Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Accidental Triplet Harvesting in Donor-acceptor Dyads with Low Spin-orbit Coupling†

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S1 Explicit solvent optimized ground state geometry of molecule 1

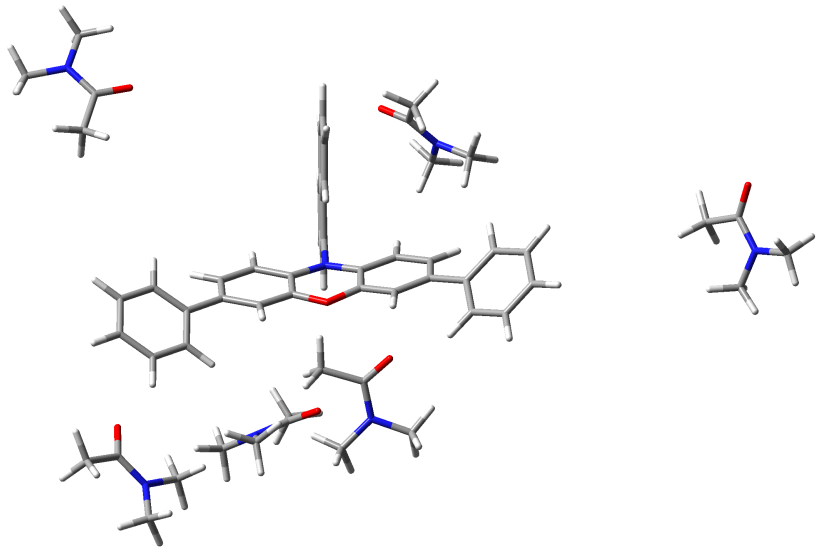

Fig S1. Optimized geometry of molecule **1** in presence of explicit DMAc solvent molecules.

S2 CASSCF converged active orbitals of molecule 1

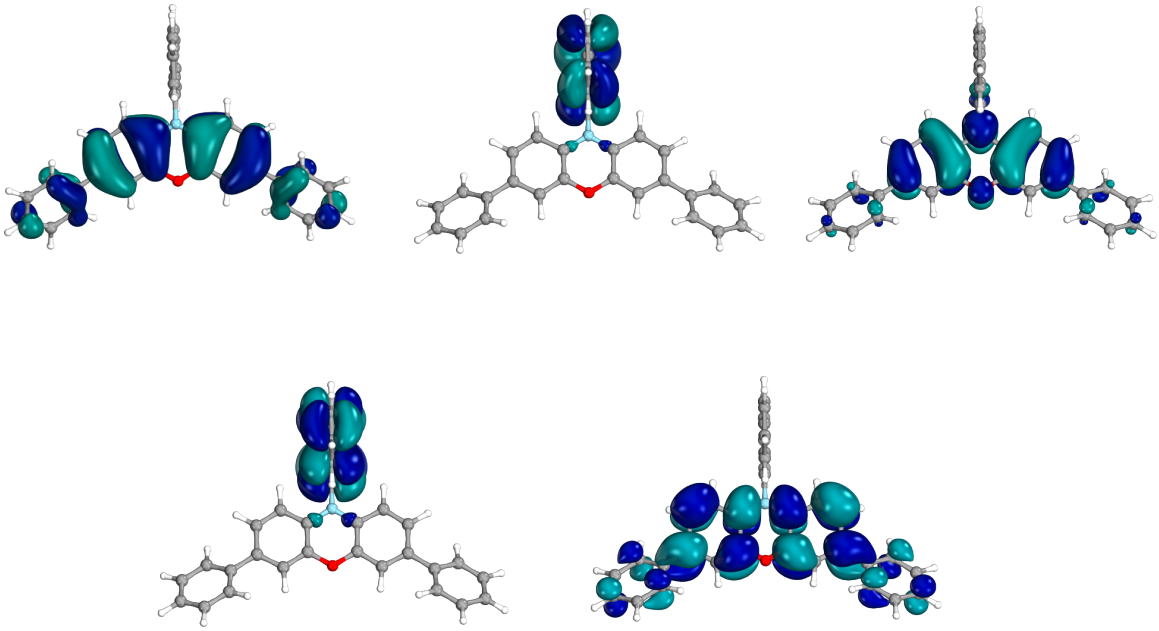

Fig S2. The state averaged (SA) CASSCF converged active orbitals are obtained by using an active space composed of six electrons distributed in 5 orbitals. 9 triplet and 10 singlet states are included in this state averaged CASSCF calculation.

S3 Computation of excitation energies, absorption wavelengths, ordering and nature of the states performed on both B3LYP and CAM-B3LYP optimized ground and first excited singlet state geometries in TD-DFT,STEOM-DLPNO-CCSD and NEVPT2 methods

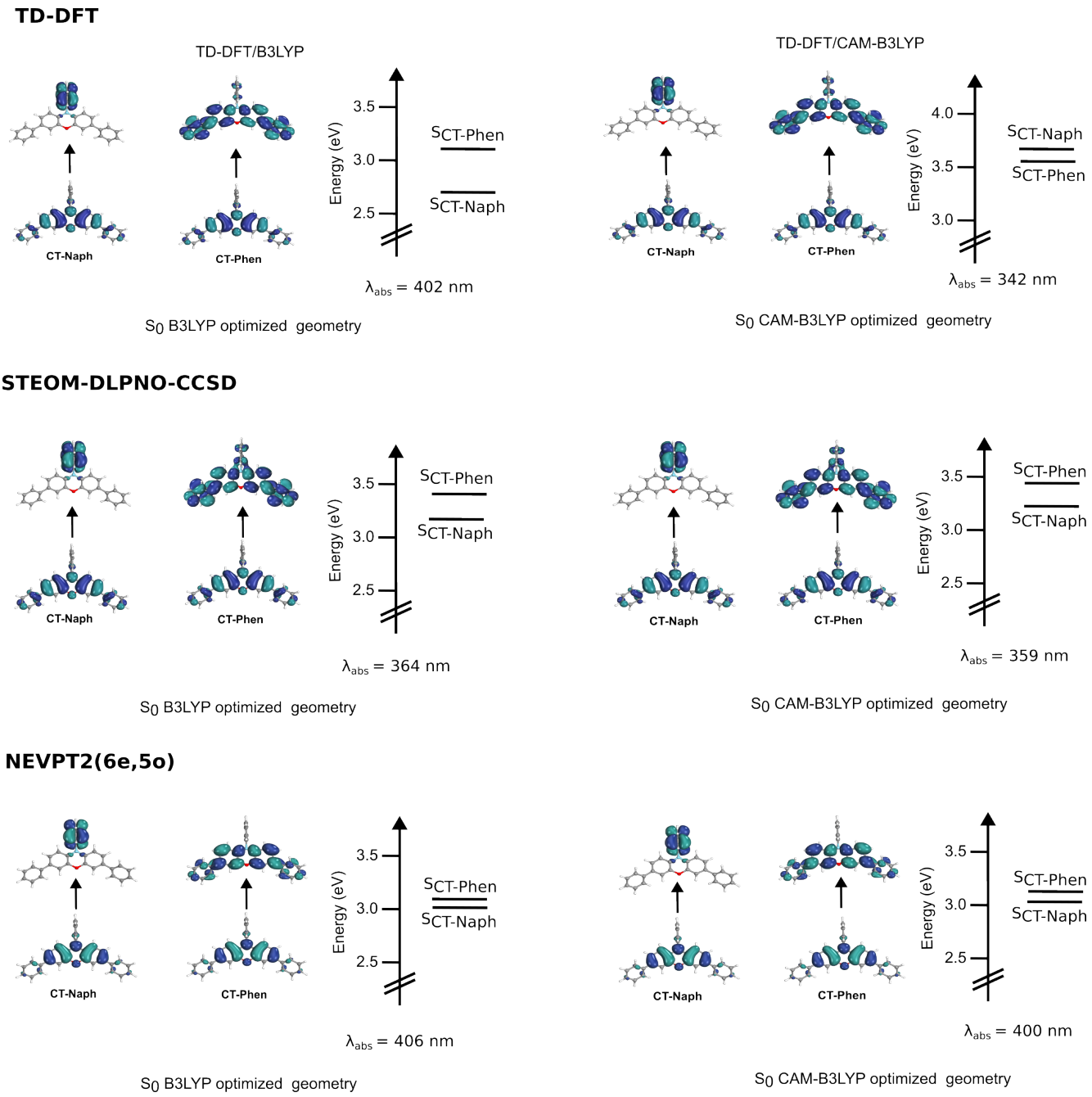

Fig S3. Excitation energies, absorption wavelengths, ordering and nature of the state in three different methods using both B3LYP and CAM-B3LYP optimized ground state geometries of molecule **1**.

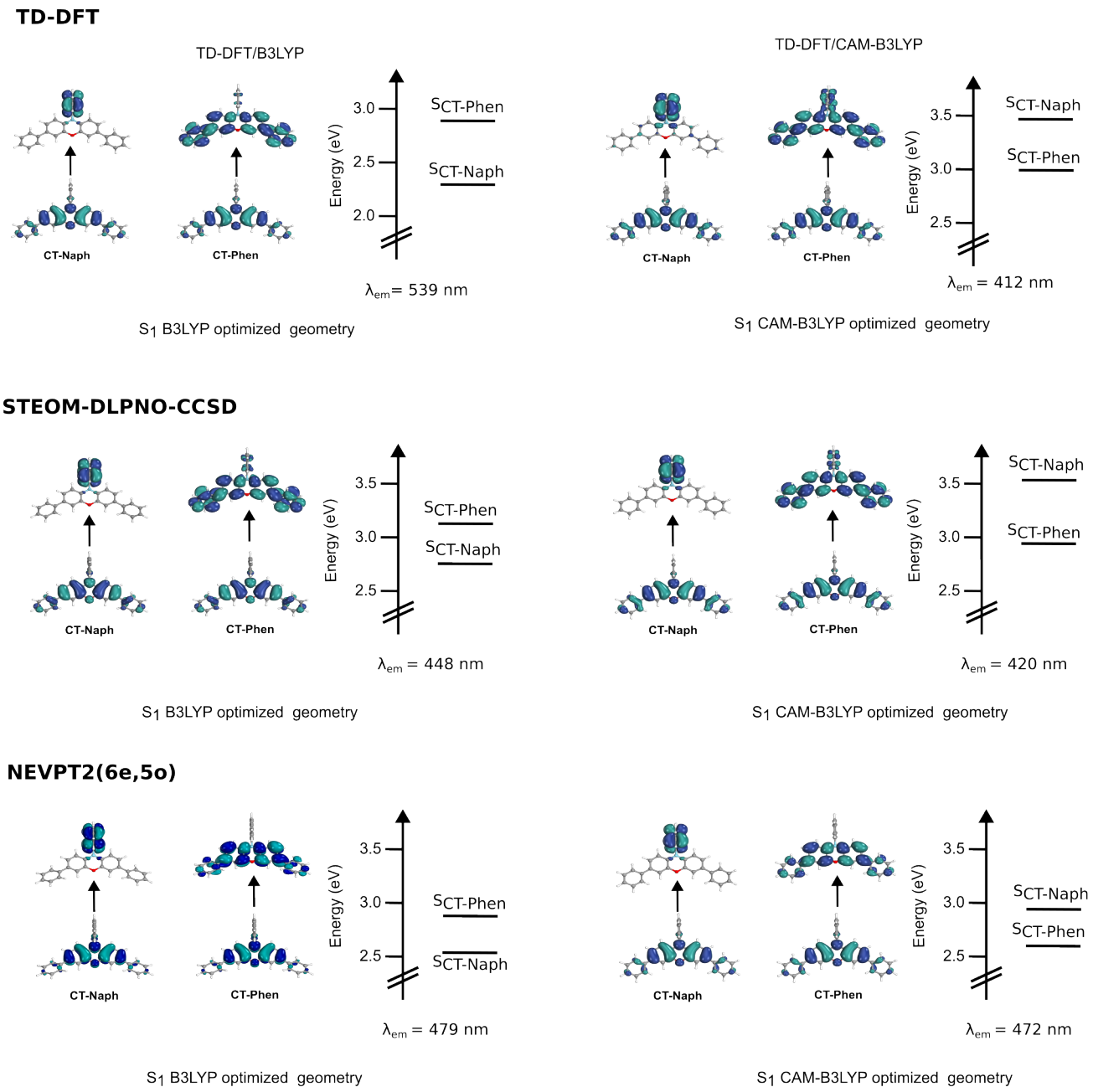

Fig S4. Excitation energies, absorption wavelengths, ordering and nature of the state in three different methods using both B3LYP and CAM-B3LYP optimized first excited singlet state geometries of molecule **1**.

S4 Analysis of Charge-transfer number of all the studied molecules

Table S1. Charge Transfer (CT) values of excited singlet and triplet electronic states of all the studied molecules at their equilibrium geometries.

state of molecule **1**	CT	state of molecule **2**	CT	state of molecule **3**	CT	state of molecule **4**	CT
$S_{CT-Naph}$	0.931	$S_{CT-Naph}$	0.951	$S_{CT-Naph}$	0.954	$S_{CT-Naph}$	0.957
$S_{CT-Phen}$	0.391	$S_{CT-Biph}$	0.477	$S_{CT-Phen}$	0.293	$S_{CT-Phen}$	0.300
$T_{CT-Phen}$	0.393	$T_{CT-Biph}$	0.318	$T_{CT-Phen}$	0.223	$T_{CT-Phen}$	0.256
$T_{CT-Naph}$	0.820	$T_{CT-Naph}$	0.941	$T_{CT-Naph}$	0.947	$T_{CT-Naph}$	0.886
$T_{LE-Naph}$	0.052	$T_{LE-Naph}$	0.041	$T_{LE-Naph}$	0.041	$T_{LE-Naph}$	0.068

To quantify the nature of the transition associated with the singlet and triplet excited electronic states, we

have performed a charge transfer (CT) analysis of all the molecules studied using TheoDore.[1] The computed CT values of each of the electronic states are given in Table S1. CT numbers greater than 0.8 for a particular state suggests that the state is associated with a strong charge-transfer character. From Table S1, it is evident that for molecule **1**, the CT number of $S_{CT-Naph}$ is 0.93 and in the other three molecules, the CT number for this state is 0.95. For the $S_{CT-Phen}$ state, the CT numbers have been found to be 0.39, 0.47, 0.29 and 0.30 in molecules **1**, **2**, **3** and **4**, respectively. Therefore, $S_{CT-Naph}$ and $S_{CT-Phen}$ are strong and weak charge transfer states, respectively. The same is true for the $T_{CT-Naph}$ and $T_{CT-Phen}$ states. On the other hand, the $T_{LE-Naph}$ state, with a very small CT value of less than 0.1, is denoted as the locally excitation (LE) state.

To understand the trend of variation of the CT and LE characters with the decrease in D-A dihedral angle from 90°, we have performed CT analysis at an interval of 4° dihedral angle up to 60° using TheoDore software. The computed CT number of molecule **1** are given in Table S2. With the decrease in D-A dihedral angle the CT number of $S_{CT-Naph}$ and $T_{CT-Naph}$ states are gradually decreased from 0.931 and 0.820 to 0.854 and 0.375, respectively. The diminishing rate of the CT number with dihedral angle is much more faster for $T_{CT-Naph}$ compared to $S_{CT-Naph}$. On the other hand, the reverse trend has been noticed for $S_{CT-Phen}$ and $T_{CT-Phen}$. The CT number of $S_{CT-Phen}$ and $T_{CT-Phen}$ vary from 0.391 to 0.407 and 0.391 to 0.489 respectively. The increasing nature of the CT values has also been seen in $T_{LE-Naph}$ state in the range of 0.052 to 0.303 with the decrease in dihedral angle. In addition, we have also performed hole and electron distribution of the excited singlet and

Table S2. Charge Transfer (CT) values of excited singlet and triplet electronic states of molecule **1** at different dihedral angle.

dihedral angle	CT of state $S_{CT-Naph}$	CT of state $T_{CT-Naph}$	CT of state $S_{CT-Phen}$	CT of state $T_{CT-Phen}$	CT of state $T_{LE-Naph}$
90.2	0.931	0.820	0.391	0.391	0.052
88	0.930	0.699	0.391	0.387	0.167
84	0.927	0.561	0.391	0.412	0.267
80	0.920	0.505	0.390	0.442	0.284
76	0.911	0.469	0.394	0.461	0.290
72	0.899	0.439	0.396	0.473	0.294
68	0.886	0.414	0.399	0.481	0.297
64	0.871	0.393	0.401	0.486	0.300
60	0.854	0.375	0.407	0.489	0.303

triplet states in order to quantify the nature of these states (CT or LE) using Multiwfn software.[2,3]. The pictorial representation of the distribution of the hole and electron of the excited singlet and triplet states are given in Fig S5. From this figure, it is clear that the hole and electron are distinctly located on two different moieties namely, phenoxazine and naphthyl respectively, indicating a strong charge-transfer character for the $S/T_{CT-naph}$ state. On the other hand, in case of $T_{LE-Naph}$ state, the hole and electron are localized on the same naphthyl part, indicating the locally-exciton (LE) type transition. The separation between hole and electron distribution of the $S/T_{CT-Phen}$ state is small which in turn implies a weak CT state. The values of D and S_r indices associated with the singlet and triplet excited states are collected in Table S3 and the results are generated from Multiwfn software. A strong CT state is defined by a large and small values of D and S_r indices, respectively, and the reverse is true for the LE state.

Table S3. The values of D and S_r indices for the excited singlet and the triplet electronic states of molecule **1** as obtained from Multiwfn software.

Transition	D ()	S_r
$S_0 \rightarrow S_{CT-Naph}$	4.15	0.15
$S_0 \rightarrow S_{CT-Phen}$	0.14	0.68
$S_0 \rightarrow T_{CT-Naph}$	2.53	0.51
$S_0 \rightarrow T_{LE-Naph}$	0.08	0.92
$S_0 \rightarrow T_{CT-Phen}$	1.23	0.67

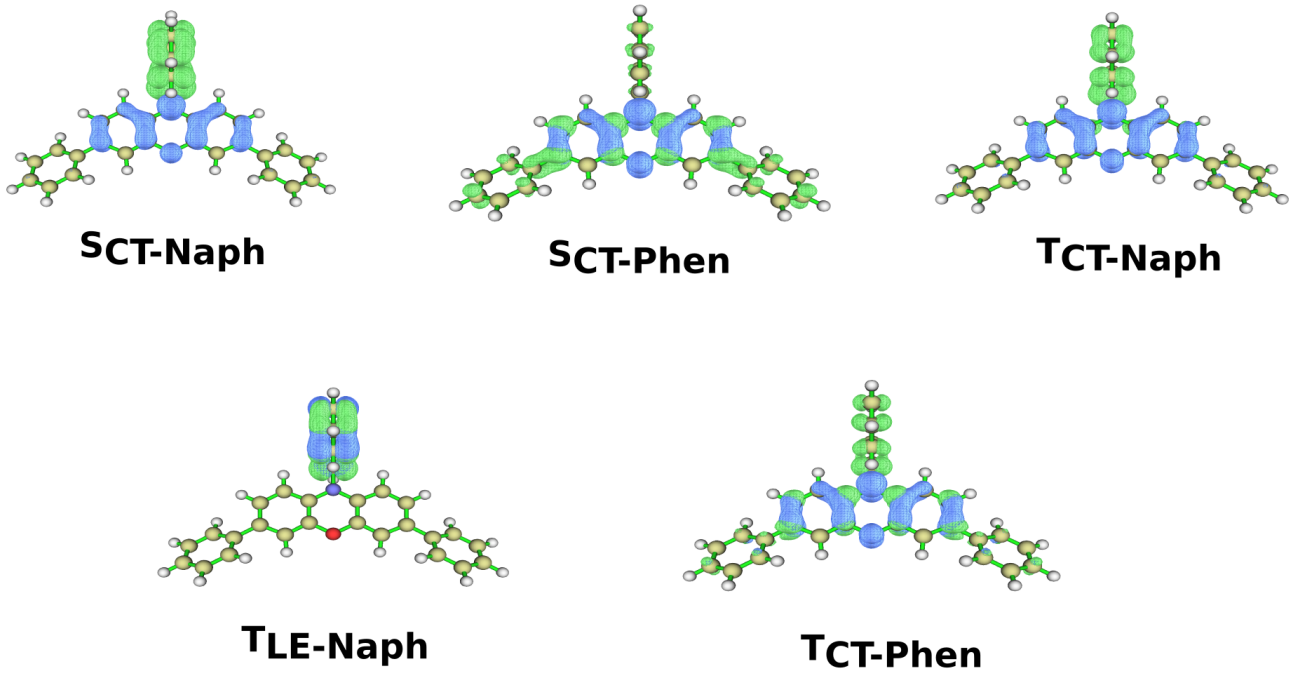

Fig S5. Hole and electron distributions of the excited singlet and triplet states of molecule **1** computed at the TD-DFT (B3LYP/6-311G(d,p)) level of theory using Multiwfn software. The blue and green color indicates the hole and electron distributions respectively.

S5 IC rate constants between $S_{CT-Phen}$ and $S_{CT-Naph}$ at various dihedral angles of molecule 1.

Table S4. k_{IC} at 300K in s^{-1} of $S_{CT-Phen} \rightsquigarrow S_{CT-Naph}$ channel and ΔE and norm of NAC vector between $S_{CT-Phen}$ and $S_{CT-Naph}$ in eV and $bohr^{-1}$.

Dihedral angle	ΔE	norm of NAC	k_{IC}
90.2	0.26	2.89	0.52×10^{11}
88	0.27	2.91	0.69×10^{11}
84	0.27	3.48	0.95×10^{11}
80	0.28	1.95	0.21×10^{11}
76	0.29	4.88	1.15×10^{11}
72	0.31	6.97	4.23×10^{11}
68	0.33	6.08	0.88×10^{11}
64	0.35	4.18	0.64×10^{11}
60	0.38	31.43	4.30×10^{12}

Table S5. SV-induced k_{ISC} of $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$ of molecule **1**

dihedral angle	ΔE (eV)	norm of NAC ($bohr^{-1}$)	k_{ISC}^{SV} (s^{-1})
68	0.12	14.63	4.32×10^{5}
64	0.06	31.76	2.67×10^{7}

It should be mentioned here that the vibronic correction to the SOC or Herzberg-Teller contribution in the determination of ISC rate is a suitable approach for the $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ pathway since direct-SOC between them is very small. In this context, following C. Marian's method,[4] we already have developed a code[5] and computed the HT contribution towards k_{ISC} for the $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ channel and the value of the corresponding rate constant is 4.49×10^{5} s^{-1} at equilibrium dihedral angle. In this case, the derivative SOC is computed for the normal mode, where the rotational motion of the naphthyl moiety across the C-N sigma bond is present. The calculated same ISC rate constant at dihedral angle of 72° has been found to be 3.18×10^{7} s^{-1}, indicating that the HT contribution is unable to meet the experimental rate constant value. It is also worth mentioning that we didn't compute the HT contribution for all the normal modes and we believe that such calculations are a bit difficult for a molecule having 171 normal modes.

S6 ISC and IC mechanisms of molecule 2

The only difference between molecules **1** and **2** is that the phenyl group attached to the phenoxazine moiety in molecule **1** is replaced by the biphenyl group in molecule **2**. The structure of molecule **2** is given in Fig S6a. The bright state of molecule **2** has $S_{CT-Biph}$ character, which is similar to the $S_{CT-Phen}$ state of **1**. The nature of the other excited states, namely ($S_{CT-Naph}$, $T_{CT-Biph}$, $T_{CT-Naph}$ and $T_{LE-Naph}$) are exactly identical to the corresponding states of molecule **1**. Similar to molecule **1**, the effect of rotation around the N-C sigma bond on the energy levels and characters of the various singlet and triplet states have been investigated for **2** and the rotation axis is depicted in Fig S6. The range of variation of the dihedral angle has been kept the same as that considered for **1**.

The nature of the CASSCF orbitals as evident from Fig S6b reveals that with the decrease in dihedral angle, the pure CT and LE states at the equilibrium geometry gain some LE and CT character, respectively. Due to orbital mixing during free rotation, the SOC among the CT-LE states start to decrease, while an opposite behavior is observed for CT-CT states and the calculated SOC values are given in Table S6. Almost similar variation of the energies of both the singlet and the triplet excited states of molecule **2** has been found as for molecule **1**. The only difference is that in molecule **2**, $T_{LE-Naph}$ and $T_{CT-Biph}$ states are located 0.03 and 0.07 eV above and below the $S_{CT-Naph}$ state at 60° whereas both the LE and the CT triplet states have placed themselves 0.004 eV lower and higher in energy with respect to $S_{CT-Naph}$, respectively. Nevertheless, all these states are energetically very close to each other in both molecules. The potential energy surfaces of the relevant singlet

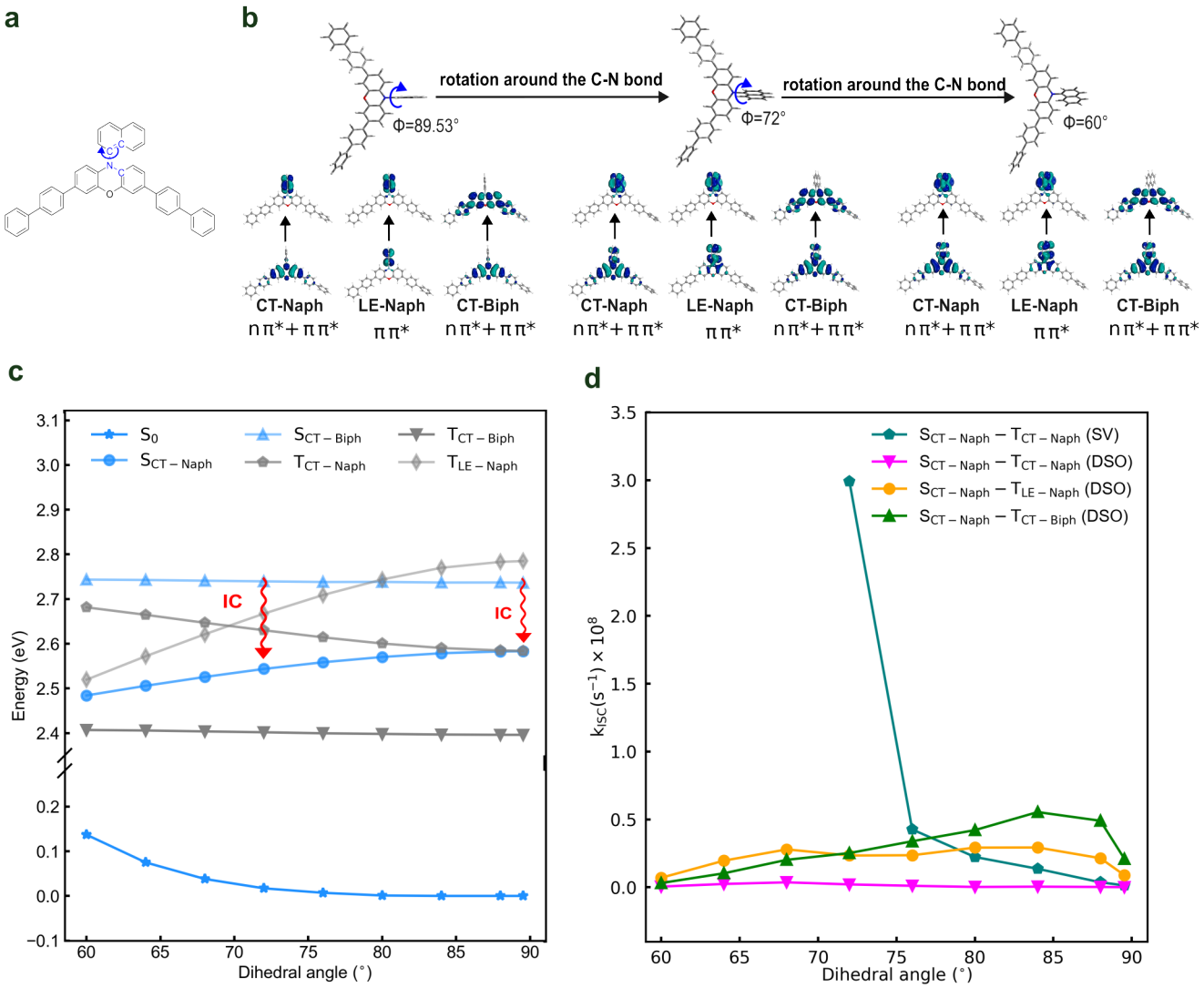

Fig S6. (a) Structure of the photoredox molecule **2** and the rotation along the C-N bond involving the dihedral angle of the C-C-N-C atoms in blue color. (b) Nature of the CASSCF orbitals involved in generation of the CT-Naph, CT-Biph and LE-Naph states and their orbital mixing with decrease in dihedral angle. (c) Potential energy surfaces of CT-Naph, CT-Biph and LE-Naph singlets and triplets states generated due to free rotation around the sigma bond.(d) Nature of variation of k_{ISC} for both DSO and SV mechanisms.

and triples states with the variation of the selected dihedral angle are depicted in Fig S6c.
In molecule **2**, the possible ISC channels are the (a) $S_{CT-Naph} \rightsquigarrow T_{CT-Biph}$, (b) $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and (c) $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$. The maximum k_{ISC} achieved with direct-SOC for (a), (b) and (c) pathways are 5.54×10^7, 2.93×10^7 and 3.63×10^6 s^{-1} at a dihedral angle 84°, 84° and 68°, respectively and can be found in Table S6.

It is to be noted that the largest DSO-aided k_{ISC} value is still lower than the experimentally observed ISC rate constant[6] (1.69×10^8 s^{-1}), indicating that the DSO only ISC mechanism is not the proper route for triplet harvesting. In this case too, the inclusion of the spin-vibronic (SV) contribution to k_{ISC} in the $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ channel helps reach a k_{ISC} value of 2.99×10^8 s^{-1}, which is in good agreement with the experimental findings. The variation of DSO and SV induced k_{ISC} with dihedral angle are depicted in Fig S6d and it is seen that at 72°, the SV-ISC rate constant in channel (c) outweighs the DSO aided k_{ISC} obtained in all of the (a), (b) and (c) pathways. The computed SV promoted k_{ISC} for the $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ pathway up to $\sim 72°$ is presented in Table S7. Earlier, it was found that free rotation induced reorganization of the various triplet states of molecule **2**[7] may lead to an increase of SOC from 0.85 cm^{-1} between $S_{CT-Naph}$ and $T_{CT-Biph}$ to 1.46 cm^{-1} between $S_{CT-Naph}$ and $T_{LE-Naph}$, indicating that SOC alone only can increase the rate constant of ISC between $S_{CT-Naph}$ and $T_{LE-Naph}$ by a factor of three compared to that between $S_{CT-Naph}$ and $T_{CT-Biph}$.

Table S6. Direct SOC induced k_{ISC} at 300K, energy gap and the magnitude of the spin-orbit coupling at different dihedral angles of molecule **2**. Here, a, b and c represent $S_{CT-Naph} \rightsquigarrow T_{CT-Biph}$, $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ transitions, respectively. The unit of k_{ISC}, ΔE and SOC are s^{-1}, eV and cm^{-1}, respectively.

Dihedral -angle	ΔE^a	SOC^a	k^a_{ISC}	ΔE^b	SOC^b	k^b_{ISC}	ΔE^c	SOC^c	k^c_{ISC}
89.53	0.18	0.87	2.10×10^7	-0.20	1.57	8.90×10^6	-0.0007	0.07	6.35×10^4
88	0.18	0.88	4.90×10^7	-0.19	1.57	2.14×10^7	-0.002	0.08	2.22×10^5
84	0.18	0.94	5.54×10^7	-0.19	1.55	2.93×10^7	-0.01	0.13	4.20×10^5
80	0.17	1.03	4.21×10^7	-0.17	1.53	2.92×10^7	-0.03	0.23	2.22×10^5
76	0.16	1.02	3.39×10^7	-0.15	1.50	2.36×10^7	-0.05	0.33	1.06×10^6
72	0.14	1.15	2.52×10^6	-0.12	1.47	2.34×10^7	-0.08	0.41	2.10×10^6
68	0.12	1.19	2.02×10^6	-0.09	1.43	2.79×10^7	-0.12	0.48	3.63×10^6
64	0.10	1.21	1.03×10^6	-0.06	1.38	1.96×10^7	-0.15	0.51	2.43×10^6
60	0.07	1.22	3.12×10^6	-0.03	1.34	7.03×10^6	-0.19	0.57	4.93×10^5

Table S7. Spin-vibronic coupling driven k_{ISC} at 300K in s^{-1} of $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ and ΔE and NAC between $T_{LE-Naph}$ and $T_{CT-Naph}$ in eV and $bohr^{-1}$ respectively.

Dihedral angle	ΔE	norm of NAC	k^{SV}_{ISC}
89.53	0.20	2.82	1.37×10^6
88	0.198	4.64	3.65×10^6
84	0.17	8.21	1.36×10^7
80	0.14	10.97	2.23×10^7
76	0.094	17.38	4.26×10^7
72	0.037	45.46	2.99×10^8

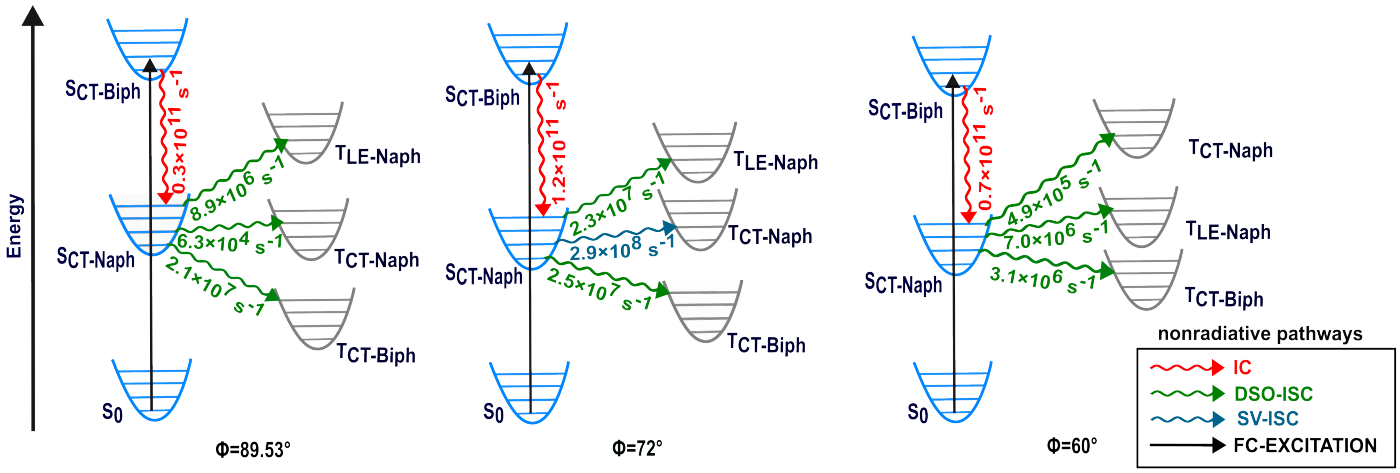

Fig S7. Schematic diagram of internal conversion (IC) and ISC mechanisms at various dihedral angles and their associated rate constants.

To examine the validity of the proposed ISC mechanism operating in molecule **2**, we have calculated the rate constant of internal conversion (IC) between the $S_{CT-Biph}$ and $S_{CT-Naph}$ states down to 60° and the corresponding data are collected in Table S8. The calculated k_{IC} values are of the order of 10^{11} and the values are quite close to the experimentally observed IC rate constant[6] (0.5×10^{11} s^{-1}) at all dihedral angles, suggesting that sufficient population transfer to the $S_{CT-Naph}$ state is possible . In particular, the value of k_{IC} at 72° is 1.22×10^{11} s^{-1} which guarantees participation of the lowest excited singlet state ($S_{CT-Naph}$) in the SV-ISC mechanism. The pictorial representation of various ISC mechanisms at three different dihedral angles are shown in Fig S7a and the trends are very similar to that found for molecule **1** in the main manuscript. The inset box in the lower right of Fig S7 contains the colors used for various nonradiative processes such as IC and ISC, and Franck-Condon excitation.

The major findings based on our theoretically evaluated nonradiative rate constants for molecules **1** and **2**

Table S8. k_{IC} at 300K in s^{-1} of $S_{CT-Biph} \rightsquigarrow S_{CT-Naph}$ channel and ΔE and NAC between $S_{CT-Phen}$ and $S_{CT-Naph}$ in eV and $bohr^{-1}$.

Dihedral angle	ΔE	norm of NAC	k_{IC}
89.53	0.153	1.83	0.34×10^{11}
88	0.154	1.85	2.84×10^{11}
84	0.158	1.86	2.52×10^{11}
80	0.168	1.84	0.93×10^{11}
76	0.17	1.89	1.11×10^{11}
72	0.19	1.94	1.22×10^{11}
68	0.21	2.01	1.22×10^{11}
64	0.23	2.07	1.20×10^{11}
60	0.25	2.12	0.72×10^{11}

elucidate the universality of the SV-ISC mechanism for the population gain in the lowest triplet state of a donor-acceptor dyad separated by a single bond.

S7 ISC mechanisms of molecule 3 and 4

Table S9. Direct SOC induced k_{ISC} at 300K, energy gap and the magnitude of the spin-orbit coupling at different dihedral angles of molecule **3**. Here, a, b and c represent $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$, $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ transitions, respectively. The unit of k_{ISC}, ΔE and SOC are s^{-1}, eV and cm^{-1}, respectively.

Dihedral angle	ΔE^a	SOC^a	k^a_{ISC}	ΔE^b	SOC^b	k^b_{ISC}	ΔE^c	SOC^c	k^c_{ISC}
89.80	0.12	0.926	2.74×10^{7}	-0.126	0.91	3.75×10^{6}	-0.002	0.08	2.02×10^{5}
88	0.12	0.917	2.55×10^{7}	-0.128	0.894	3.16×10^{6}	-0.002	0.11	3.65×10^{5}
84	0.118	0.907	2.69×10^{7}	-0.116	0.890	4.15×10^{6}	-0.01	0.18	1.27×10^{6}
80	0.113	0.904	2.56×10^{7}	-0.092	0.888	3.28×10^{6}	-0.03	0.25	1.57×10^{6}
78	0.109	0.911	2.18×10^{7}	-0.077	0.879	2.41×10^{6}	-0.04	0.28	4.85×10^{6}
76	0.10	0.901	1.66×10^{7}	-0.063	0.881	1.59×10^{6}	-0.056	0.31	0.74×10^{6}
72	0.084	0.911	0.86×10^{7}	-0.029	0.884	2.53×10^{6}	-0.09	0.37	3.77×10^{5}
68	0.058	0.909	3.13×10^{6}	0.003	0.896	0.68×10^{6}	-0.12	0.42	1.27×10^{5}
64	0.039	0.917	1.89×10^{6}	0.034	0.931	0.94×10^{6}	-0.16	0.47	3.24×10^{5}
60	-0.002	0.899	8.73×10^{5}	0.053	0.981	1.13×10^{6}	-0.19	0.54	5.09×10^{5}

Table S10. Spin-vibronic coupling driven k_{ISC} of molecule **3** at 300K in s^{-1} of $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ and ΔE and NAC between $T_{LE-Naph}$ and $T_{CT-Naph}$ in eV and $bohr^{-1}$ respectively.

Dihedral angle	ΔE	norm of NAC	k^{SV}_{ISC}
89.80	0.124	4.80	0.64×10^{5}
88	0.126	4.83	0.71×10^{5}
84	0.104	6.83	2.41×10^{5}
80	0.062	13.11	1.95×10^{6}
78	0.034	28.08	1.12×10^{7}
76	0.007	148.66	5.11×10^{8}

In addition to molecules **1** and **2**, the other two important D-A molecules investigated here also support our proposed accidental triplet harvesting mechanism. The structure of these two molecules (**3** and **4**) and the rotation axes are shown in Figs S8a and S10a, respectively. We find that the nature of the excited singlet and triplet states obtained upon photoexcitation are the same as those of **1** and **2** and the relevant excitation characters are depicted in Figs S8b and S10b. For both **3** and **4**, the variation of the relative energies of the excited electronic states (singlet and triplets) due to the rotation around the C-N sigma bond are shown in Figs S8c and S10c. From these figures, the only significant change that can be noted is the rapid decrease

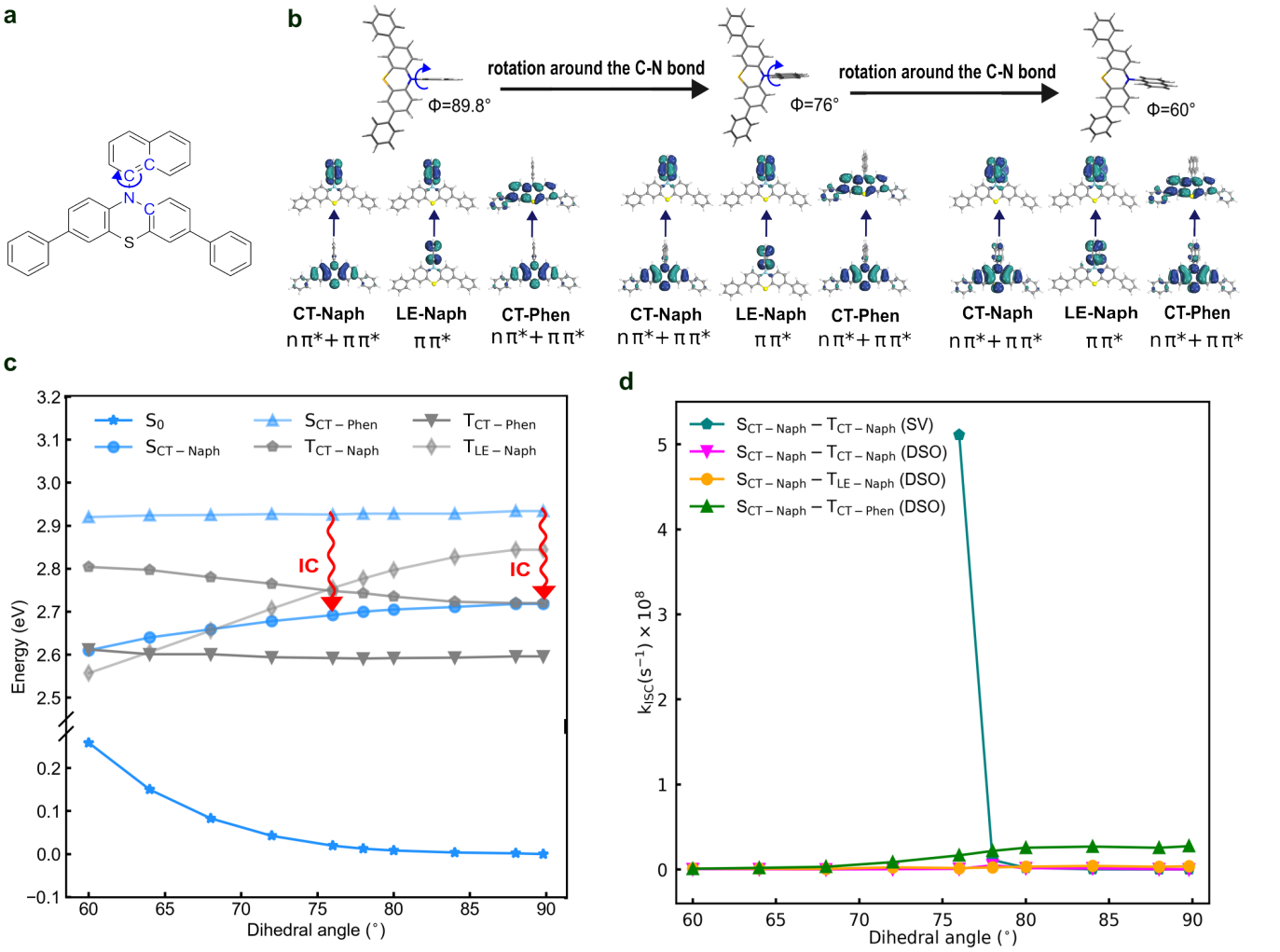

Fig S8. (a) Structure of the photoredox molecule **3** and the rotation along the C-N bond involving the dihedral angle of the C-C-N-C atoms in blue color. (b) Nature of the CASSCF orbitals involved in generation of the CT-Naph, CT-Phen and LE-Naph states and their orbital mixing with decrease in dihedral angle. (c) Potential energy surfaces of CT-Naph, CT-Phen and LE-Naph singlets and triplets states generated due to free rotation around the sigma bond.(d) Nature of variation of k_{ISC} for both DSO and SV mechanisms.

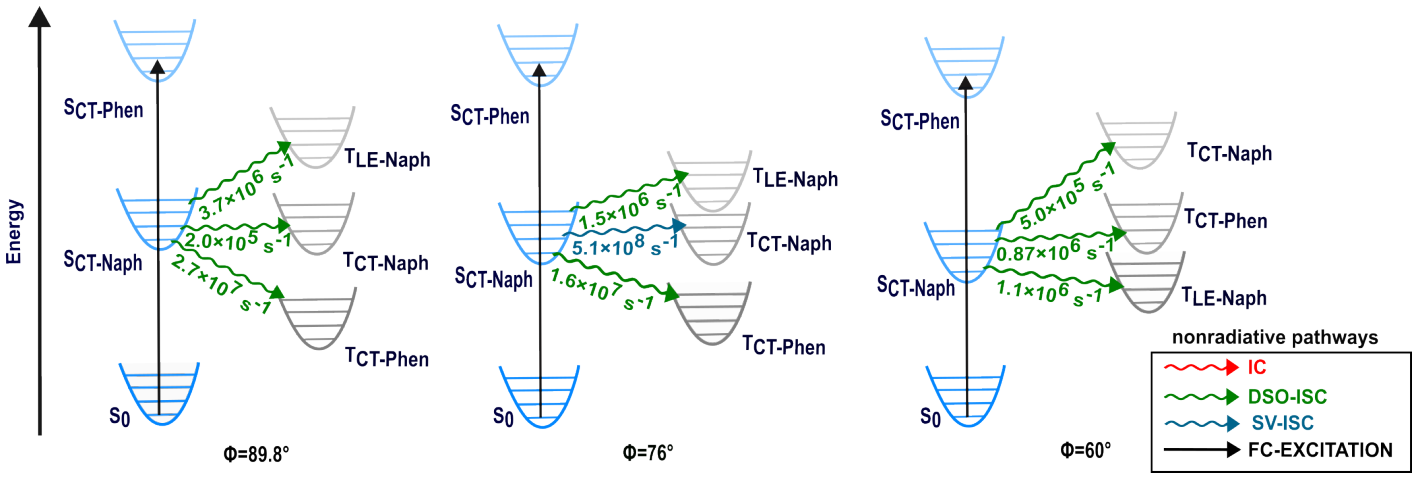

Fig S9. Schematic diagram of ISC mechanisms of molecule **3** at various dihedral angles and their associated rate constants.

of energy of the $T_{LE-Naph}$ state and as a consequence, the potential energy curves of $T_{LE-Naph}$ crosses $T_{CT-Naph}$ and $S_{CT-Naph}$ at earlier dihedral angles compared to what was observed in molecules **1** and **2**. Interestingly, the possible ISC pathways in both **3** and **4** are also identical to what has been seen in **1**. The energy gap, direct-SOC

and the associated rate constants of all three probable pathways are also provided in Tables S9 and S11. The computed rate constants indicate that none of the possible DSO-assisted ISC pathways are capable of reaching the experimental ISC rate constants of 1.7-2.3$\times10^8$ and 1.5-1.8$\times10^8$ s^{-1} for **3** and **4**, respectively.[8] However, after incorporating the effect of the SV part into the the expression of k_{ISC} along the $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ pathway of molecules **3** and **4**, the rate constants have increased substantially and the corresponding values have been found to be 5.11$\times10^8$ and 1.67$\times10^8$ s^{-1}, respectively. Overall, the calculated results corroborate well with the experimental findings. We also note that in molecules **3** and **4**, the largest SV-aided k_{ISC} are found at dihedral angles of 76° and 78°, respectively. The variation of the DSO and the SV-induced ISC rate constants at various dihedral angles for both molecules are shown in Figs S8d and S10d. The computed SV-guided ISC rate constants are also presented in Tables S10 and S12. Pictorial representations of DSO- and SV-favored ISC routes and their associated rate constants at three different dihedral angles are also depicted in Figs S9 and S11. From these theoretical findings, we can infer that all the molecules studied follow the free rotation induced accidental SV mechanism to ensure efficient triplet harvesting process.

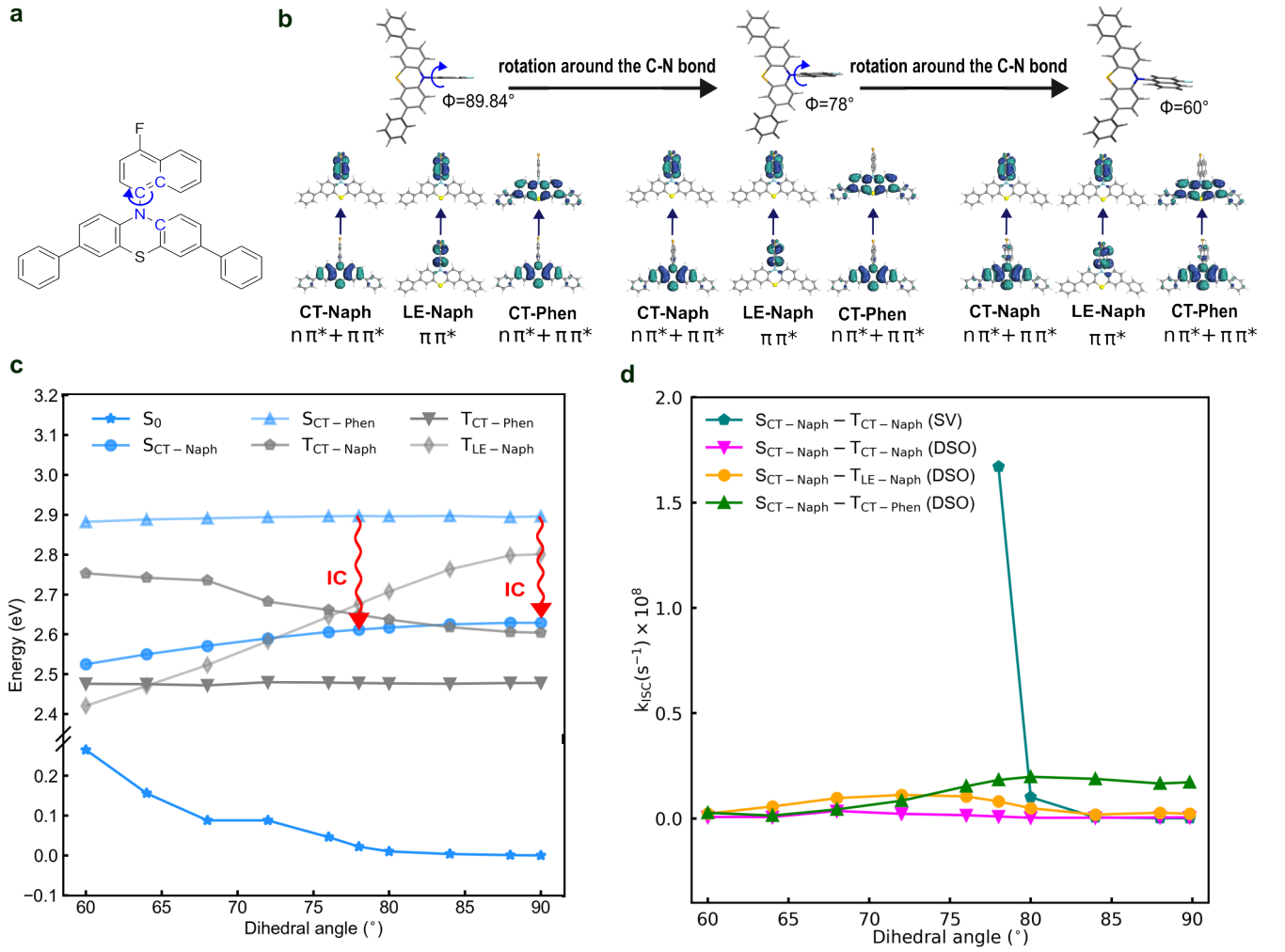

Fig S10. (a) Structure of the photoredox molecule **4** and the rotation along the C-N bond involving the dihedral angle of the C-C-N-C atoms in blue color. (b) Nature of the CASSCF orbitals involved in generation of the CT-Naph, CT-Phen and LE-Naph states and their orbital mixing with decrease in dihedral angle. (c) Potential energy surfaces of CT-Naph, CT-Phen and LE-Naph singlets and triplets states generated due to free rotation around the sigma bond.(d) Nature of variation of k_{ISC} for both DSO and SV mechanisms.

Table S11. Direct SOC induced k_{ISC} at 300K, energy gap and the magnitude of the spin-orbit coupling at different dihedral angles of molecule **4**. Here, a, b and c represent $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$, $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ transitions, respectively. The unit of k_{ISC}, ΔE and SOC are s^{-1}, eV and cm^{-1}, respectively.

Dihedral angle	ΔE^a	SOC^a	k^a_{ISC}	ΔE^b	SOC ^{b}	k^b_{ISC}	ΔE^c	SOC ^{c}	k^c_{ISC}
89.84	0.151	0.851	1.72×10^7	-0.172	0.724	2.26×10^6	0.025	0.167	5.32×10^5
88	0.151	0.841	1.66×10^7	-0.169	0.722	2.71×10^6	0.023	0.169	5.19×10^5
84	0.149	0.858	1.88×10^7	-0.138	0.715	1.85×10^6	0.007	0.206	3.67×10^5
80	0.14	0.879	1.98×10^7	-0.09	0.699	4.90×10^6	-0.02	0.252	3.49×10^5
78	0.134	0.893	1.83×10^7	-0.064	0.702	0.81×10^7	-0.037	0.270	9.47×10^5
76	0.127	0.908	1.53×10^7	-0.038	0.700	1.05×10^7	-0.055	0.287	1.57×10^6
72	0.11	0.943	0.84×10^7	0.007	0.709	1.12×10^7	-0.092	0.33	2.21×10^6
68	0.099	0.953	4.31×10^6	0.048	0.724	0.96×10^7	-0.164	0.40	3.58×10^6
64	0.075	1.01	1.39×10^6	0.079	0.766	5.72×10^6	-0.192	0.38	0.73×10^6
60	0.049	1.05	2.71×10^6	0.104	0.829	2.28×10^6	-0.228	0.41	0.72×10^6

Table S12. Spin-vibronic coupling driven k_{ISC} of molecule **4** at 300K in s^{-1} of $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ and ΔE and NAC between $T_{LE-Naph}$ and $T_{CT-Naph}$ in eV and $bohr^{-1}$ respectively.

Dihedral angle	ΔE	norm of NAC	k^{SV}_{ISC}
89.84	0.197	2.99	0.99×10^5
88	0.192	3.14	1.15×10^5
84	0.145	4.94	5.61×10^5
80	0.07	12.50	1.01×10^7
78	0.027	35.68	1.67×10^8

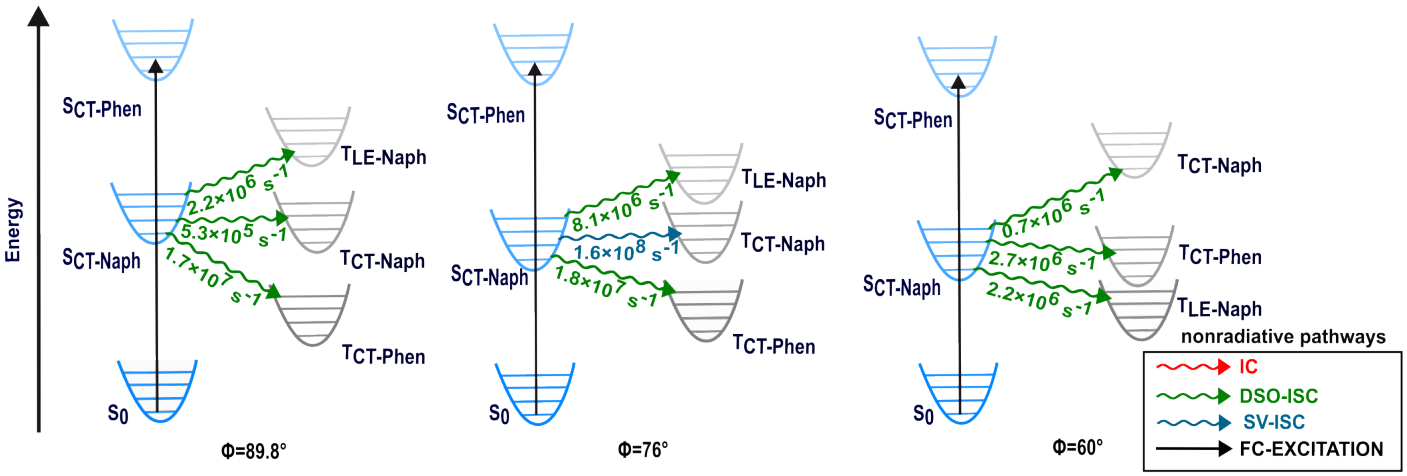

Fig S11. Schematic diagram of ISC mechanisms of molecule **4** at various dihedral angles and their associated rate constants.

S8 Discussion about the Duschinsky rotation matrix (J) and displacement vector (D)

Upon photoexcitation from the ground to the excited electronic state, the normal mode coordinates of the excited state gets displaced and rotated with respect to the ground state. This is true for any pair of initial and final electronic states. If the normal mode coordinates of the initial and final electronic states are represented by $\mathbf{Q}_i$ and $\mathbf{Q}_f$, respectively, the connection between these two coordinates is described by the following relation

$$\mathbf{Q}_f = \sum_i \mathbf{J}_{if}\mathbf{Q}_i + \mathbf{D}_f, \tag{S1}$$

where **J** and **D** are the Duschinsky rotation matrix and displacement vectors, respectively. **J** is a unit less matrix whereas **D** can be expressed in massweighted coordinate with units of $(\text{amu})^{0.5}$ as

$$\mathbf{D} = \mathbf{L}\sqrt{m}(r - r') \tag{S2}$$

The graphical representation of the relation between the normal-mode coordinates of the ground and excited

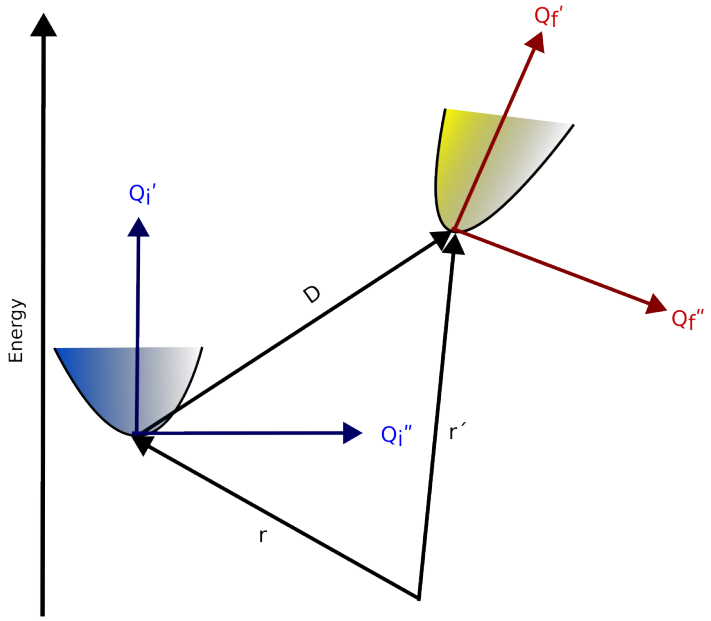

Fig S12. Relation between the normal mode coordinates of the initial and the final electronic state in terms of rotation and displacement.

electronic states is shown in Fig S12. Here, $\mathbf{Q}'$ and $\mathbf{Q}''$ represents the coordinates of the normal mode of the initial and final electronic states, respectively. r and r′ denotes the Cartesian displacements of the initial and final states, respectively, with respect to a reference point. **L** is the eigenvector matrix obtained after diagonalizing the mass-weighted Cartesian force constant matrix and m indicates the mass of the nuclei. **D** is simply the translatipn of the final state with respect to that of initial state. **J** on the other hand rotates the normal coordinates of the final electronic state with respect to that of the initial state. **J** is a unitary matrix and thus in principle, the determinant of this matrix should be one. However, a large number of off-diagonal elements may be found if the vibrational and the rotational motions are coupled as has been observed for geometries with significant change in different structural parameters such as dihderal angles, bond angles and bond lengths. In this situation, the determinant of **J** will deviate from 1. The off-diagonal elements of the Duschinsky rotation matrix actually indicate the coupling between normal modes of two different electronic states. The larger the off-diagonal elements, the higher will the coupling between them be. Usually, a small energy gap and large SOC play dominant roles in determining the values of k_{ISC} rate constant. However, when vibrational effects are taken into account in the computation of any nonradiative rate constants, the Duschinsky rotation matrix and displacement vectors appear automatically and they often also play important roles. For example, the displacement vector may change the value of k_{ISC} by two orders of magnitude for fluorenone while the Duschinsky rotation and displacement vector may alter the rate constant of ISC of benzophenone by

one order of magnitude.[9]. It has also been found that for an energy gap less than 0.7 eV between the singlet and the triplet states, the ISC rate constant without Duschinsky rotation is decreased by one to three orders magnitude.[10]

S9 k_{ISC}^{DSO} values at 300K for all three pathways of molecules 1 and 2 with or without incorporating the effect of Duschinsky rotation matrix (J) and displacement vector (D) at different dihedral angles

Table S13. a,b and c represent k_{ISC}^{DSO} of $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$, $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ transitions, respectively, with I and II indicate without inclusion of Duschinsky rotation matrix (**J**) and displacement vector (**D**) respectively. The unit of k_{ISC}, ΔE and SOC are s^{-1}, eV and cm^{-1}, respectively.

Dihedral angle	$k_{ISC}^{a,I}$	$k_{ISC}^{a,II}$	$k_{ISC}^{b,I}$	$k_{ISC}^{b,II}$	$k_{ISC}^{c,I}$	$k_{ISC}^{c,II}$
90.2	3.21×10^{7}	3.80×10^{6}	4.06×10^{5}	6.07×10^{7}	6.29×10^{5}	5.11×10^{6}
88	3.57×10^{7}	1.34×10^{6}	9.98×10^{5}	6.43×10^{7}	8.65×10^{5}	7.03×10^{6}
84	4.16×10^{7}	3.47×10^{6}	2.12×10^{6}	3.04×10^{7}	1.89×10^{6}	1.48×10^{7}
80	3.86×10^{7}	3.17×10^{7}	4.02×10^{6}	2.95×10^{7}	3.23×10^{6}	2.24×10^{7}
76	2.48×10^{7}	2.75×10^{7}	7.77×10^{6}	3.47×10^{7}	3.55×10^{6}	1.98×10^{7}
72	7.08×10^{6}	4.21×10^{7}	1.37×10^{7}	7.86×10^{7}	5.03×10^{6}	2.45×10^{7}
68	2.35×10^{6}	4.11×10^{7}	4.79×10^{6}	5.78×10^{7}	2.97×10^{6}	2.89×10^{7}
64	4.54×10^{6}	4.82×10^{7}	1.64×10^{7}	7.61×10^{7}	6.49×10^{5}	6.08×10^{6}
60	4.00×10^{6}	5.09×10^{7}	3.50×10^{6}	8.07×10^{7}	3.81×10^{5}	3.54×10^{5}

The detailed discussion of the influence of the Duschinsky rotation matrix and displacement vector on the intersystem crossing rate of molecule **1** are provided in the main manuscript and the computed rate constants are given in Table S13.

Table S14. a,b and c represent k_{ISC}^{DSO} of $S_{CT-Naph} \rightsquigarrow T_{CT-Biph}$, $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ transitions, respectively, with I and II indicate without inclusion of Duschinsky rotation matrix (**J**) and displacement vector (**D**) respectively. The unit of k_{ISC}, ΔE and SOC are s^{-1}, eV and cm^{-1}, respectively.

Dihedral angle	$k_{ISC}^{a,I}$	$k_{ISC}^{a,II}$	$k_{ISC}^{b,I}$	$k_{ISC}^{b,II}$	$k_{ISC}^{c,I}$	$k_{ISC}^{c,II}$
89.53	3.57×10^{7}	1.82×10^{7}	5.20×10^{4}	3.86×10^{7}	1.58×10^{5}	1.14×10^{6}
88	8.11×10^{7}	3.67×10^{7}	1.86×10^{5}	1.38×10^{8}	4.50×10^{5}	3.09×10^{6}
84	9.44×10^{7}	5.11×10^{7}	2.27×10^{6}	1.18×10^{8}	1.12×10^{6}	1.25×10^{7}
80	8.67×10^{7}	4.21×10^{7}	5.79×10^{6}	6.43×10^{7}	5.92×10^{5}	2.16×10^{7}
76	5.08×10^{7}	4.74×10^{7}	1.36×10^{7}	1.61×10^{7}	3.89×10^{5}	2.10×10^{7}
72	2.67×10^{7}	5.07×10^{7}	2.95×10^{7}	7.73×10^{7}	2.58×10^{6}	1.85×10^{7}
68	2.76×10^{6}	6.21×10^{7}	1.78×10^{7}	1.41×10^{8}	1.91×10^{6}	8.01×10^{6}
64	1.29×10^{7}	6.07×10^{7}	5.25×10^{7}	1.76×10^{8}	8.04×10^{6}	3.24×10^{6}
60	4.60×10^{6}	4.36×10^{7}	7.14×10^{6}	1.43×10^{8}	2.82×10^{6}	3.37×10^{4}

In molecule **2**, the role of J and D on k_{ISC} in all three pathways, (a),(b) and (c) are the same as that already observed for **1**. The relevant results for **2** are also provided in Table S14.

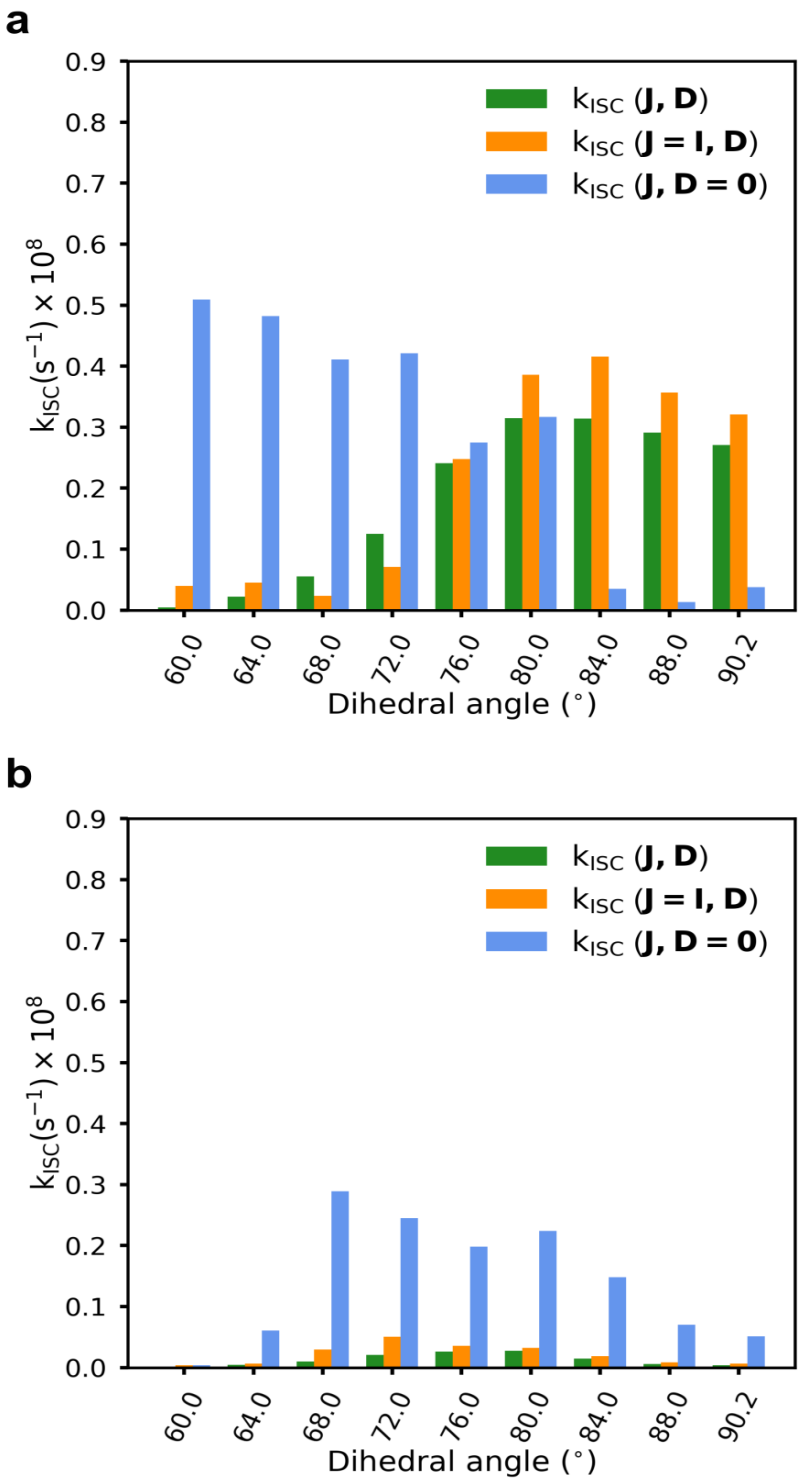

Fig S13. Effect of Duschinsky rotation matrix (**J**) and displacement vectors (**D**) on k_{ISC}^{DSO} of (a) $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$ and (b) $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ channels of molecule **1**.

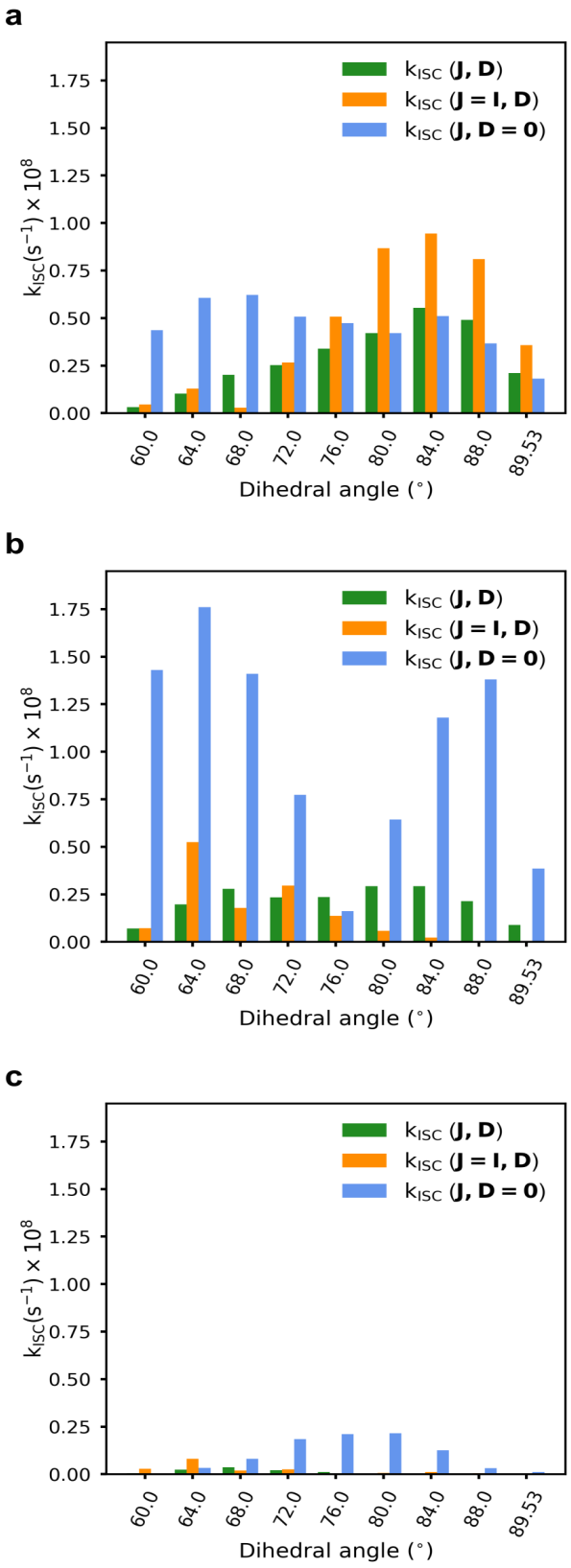

Fig S14. Effect of Duschinsky rotation matrix (**J**) and displacement vectors (**D**) on k_{ISC}^{DSO} of (a) $S_{CT-Naph} \rightsquigarrow T_{CT-Biph}$, b) $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ and (c) $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$ channels of molecule **2**.

S10 Effect of basis set on the spin-orbit coupling matrix elements

We have also computed the SOC with the def2-SVP basis set on the first excited singlet state geometry of 10-(naphthalen-1-yl)-3,7-diphenyl-10H-phenoxazine. No significant changes have been observed. The computed SOC values among $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$, $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$ and $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ with def2-TZVP and def2-SVP basis sets are given in Table S12.

Table S15. Spin-orbit coupling in cm^{-1} between $S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$, $S_{CT-Naph} \rightsquigarrow T_{CT-Phen}$ and $S_{CT-Naph} \rightsquigarrow T_{LE-Naph}$ transitions in two different basis set of molecule **1**.

basis set	$S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$	$S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$	$S_{CT-Naph} \rightsquigarrow T_{CT-Naph}$
def2-SVP	0.11	1.54	0.87
def2-TZVP	0.14	1.59	0.91

S11 Effect of solvent polarity on the energetic ordering of the excited states

We have computed the excitation energies of the singlet and triplet excited states (CT-Nap, LE-Naph and CT-Phen) in toluene, using both the equilibrium geometries of S_0 and $S_{CT-Naph}$ of 10-(naphthalen-1-yl)-3,7-diphenyl-10H-phenoxazine. Also in this case, the positions of the excited singlet and triplet states on the energetic scale remain practically unchanged (Fig S15) with respect to the corresponding results obtained with DMAc solvent, indicating that the solvent polarity hardly has any effect on the absorption and emission wavelengths. Although ISC rate is largely unaffected in different solvents, ISC quantum yield may be influenced by the solvent polarity.

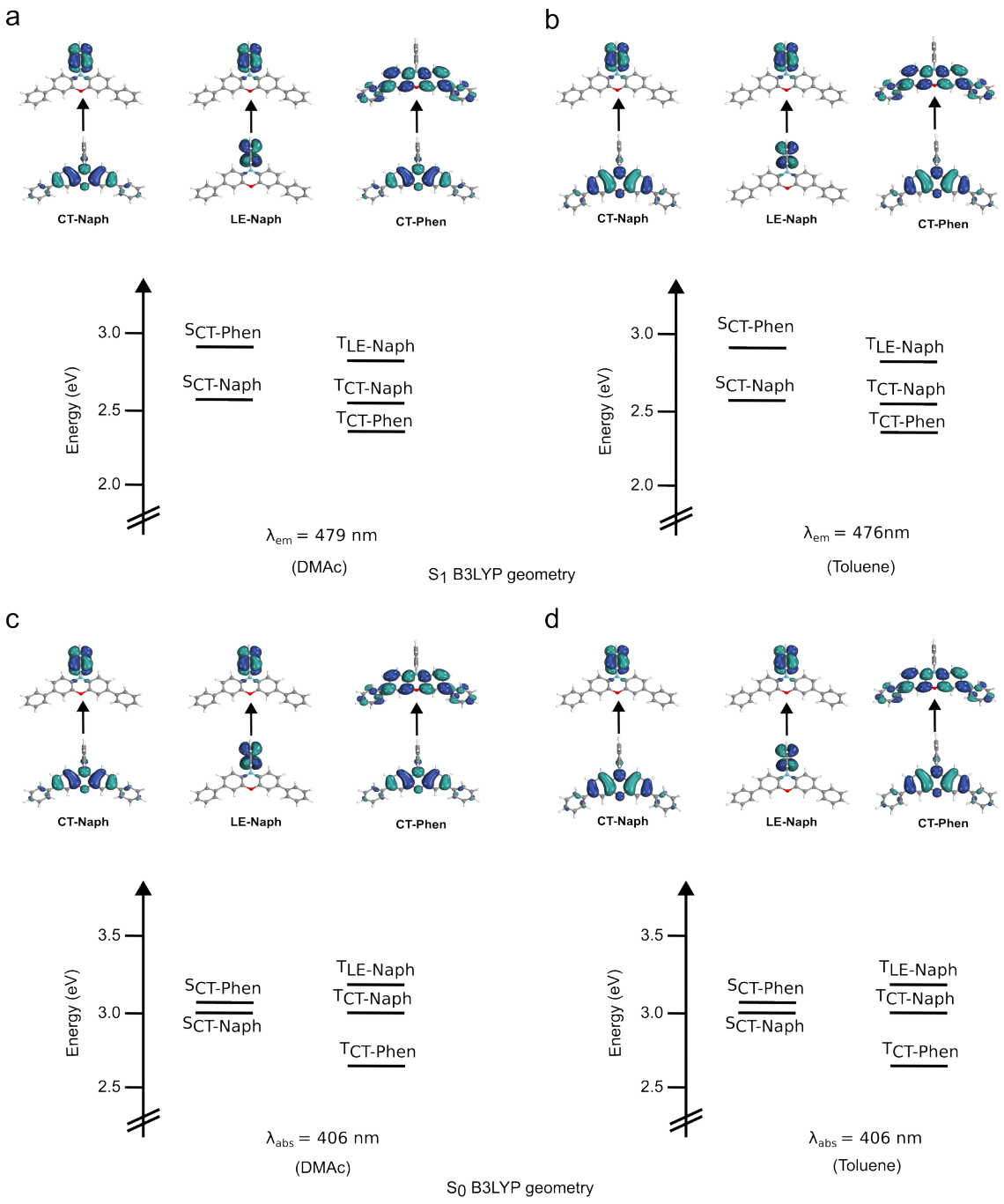

Fig S15. The energetic ordering of the excited singlet and triplet states in (a) DMAc and (b) toluene solvents of molecule 10-(naphthalen-1-yl)-3,7-diphenyl-10H-phenoxazine computed at the NEVPT2 level of theory.

S12 Nature of the mode-specific NACMEs

The normal mode specific nonadiabatic coupling matrix element (NACME) between two singlets or two triplets can be expressed as,

$$\langle \mathrm{S/T_{CT/LE}}|\frac{\partial}{\partial \mathbf{Q}_k}|\mathrm{S/T_{CT/LE}}\rangle = \frac{\langle \mathrm{S/T_{CT/LE}}|\frac{\partial V}{\partial \mathbf{Q}_k}|\mathrm{S/T_{CT/LE}}\rangle}{E_{\mathrm{S/T_{CT/LE}}} - E_{\mathrm{S/T_{CT/LE}}}} \tag{S3}$$

Here, V and $\mathbf{Q}_k$ are the nulceus-electron attraction operator and the normal coordinate of the k-th mode, respectively. The transformation of the NAC from Cartesian space to the normal mode specific coordinate has been done following Refs. 11,12. The energies of the singlet or triplet states having CT/LE character is defined by $E_{\mathrm{S/T_{CT/LE}}}$. These nonadiabatic coupling matrix element depends upon two factors: the derivative term in the numerator and the energy gap between the two singlet or two triplet states as found in the denominator of eqn (S3). We note that the dependence of the NAC on the factor appearing in the numerator is not straightforward. For our purposes, we have computed the NAC in the singlet manifold between $\mathrm{S_{CT-Phen/CT-Biph}}$ and $\mathrm{S_{CT-Naph}}$ states for the calculation of $\mathrm{k_{IC}}$ at all the dihedral angles down to 60° while in the triplet manifold, $\mathrm{k_{IC}}$ between $\mathrm{T_{LE-Naph}}$ and $\mathrm{T_{CT-Naph}}$ has been calculated within the range of $90° - 72°$. From Fig 1c (main manuscript) and Fig S6c, it is evident that the energy gap between $\mathrm{T_{LE-Naph}}$ and $\mathrm{T_{CT-Naph}}$ decreases due to the change in the dihedral angle from 90° to 72° and this is true for both molecules **1** and **2**. Interestingly, this decreasing trend helps increase the magnitude of the norm of the NAC vector and mode-specific NACMEs, and the corresponding findings are reflected in the data in Tables 2 (main manuscript) and S7 and Figs S16 and S17. The nature of the variation of the mode-specific NACMEs between $\mathrm{S_{CT-Phen/Biph}}$ and $\mathrm{S_{CT-Naph}}$ with dihedral angle for both **1** and **2** are given in Figs S18 and S19, respectively.

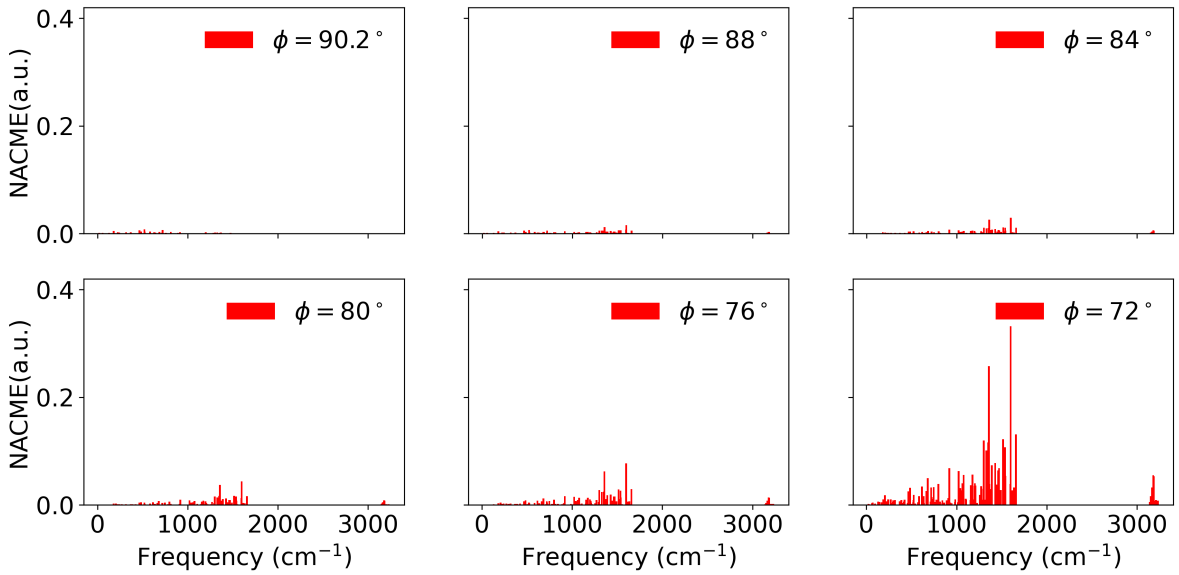

Fig S16. Mode specific NACMEs between the $\mathrm{T_{LE-Naph}}$ and $\mathrm{T_{CT-Naph}}$ of molecule **1**.

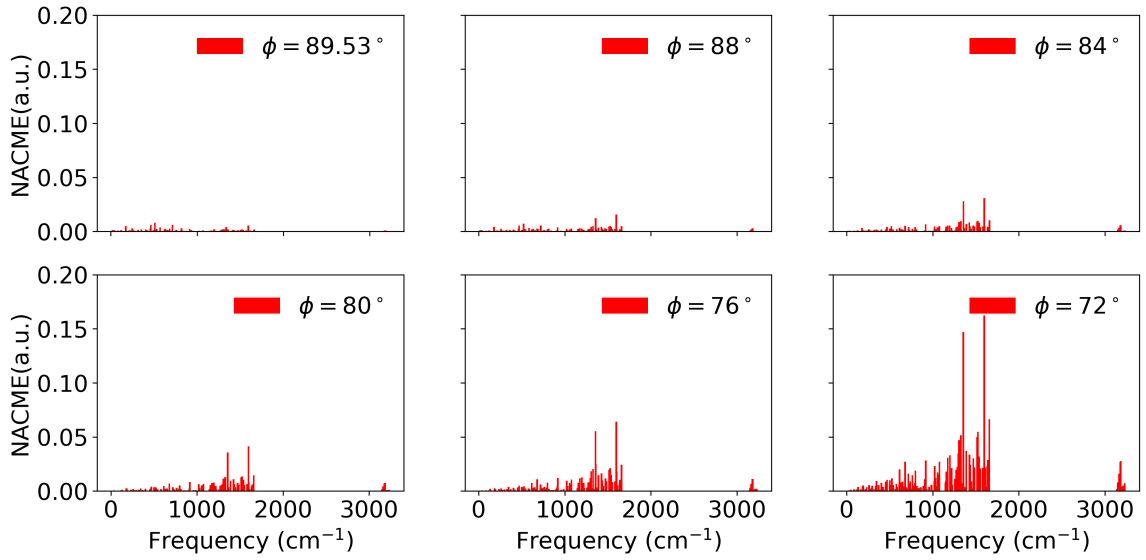

Fig S17. Mode specific NACME among $T_{LE-Naph}$ and $T_{CT-Naph}$ states of molecule **2**.

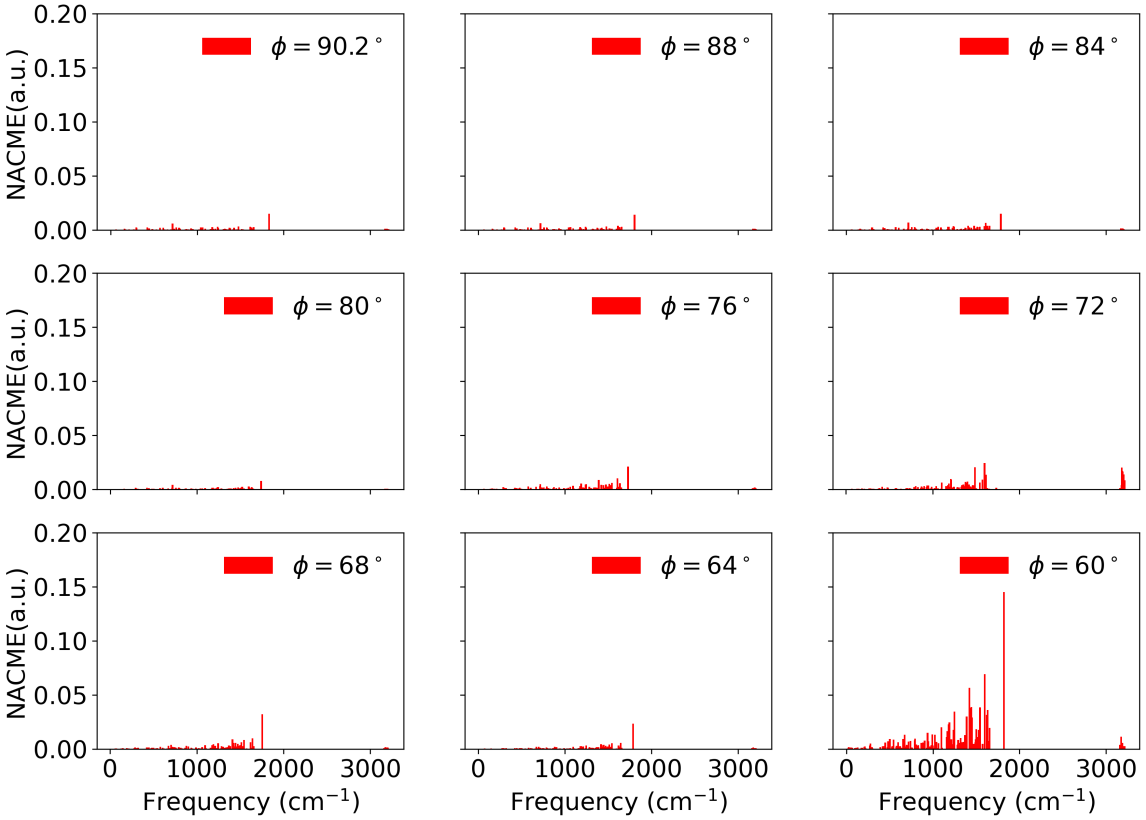

Fig S18. Mode specific NACMEs between the $S_{CT-Phen}$ and $S_{CT-Naph}$ of molecule **1**.

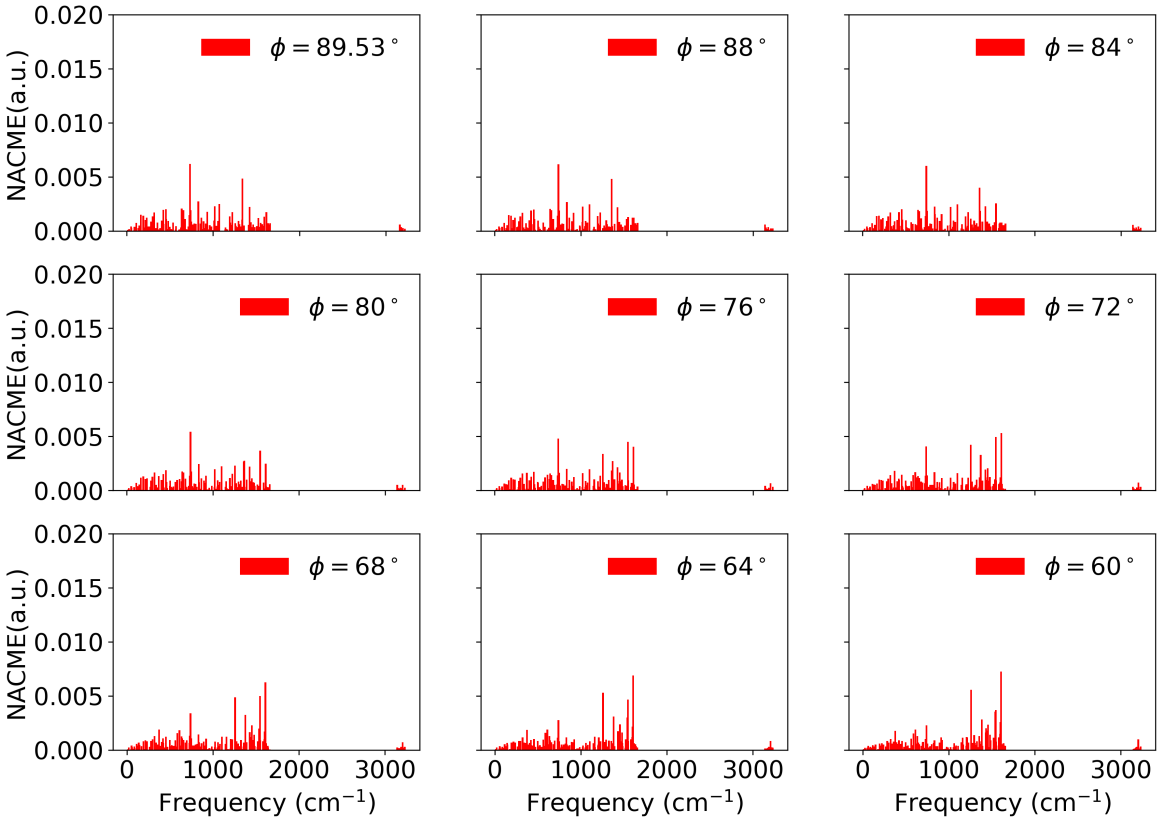

Fig S19. Mode specific NACME among $S_{CT-Biph}$ and $S_{CT-Naph}$ states of molecule **2**.

S13 Frequencies of all geometries of molecule 1 computed at (B3LYP/6-311G(d,p)) level of theory

molecule-1						
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 90.2^\circ$)	$\omega_{S_{CT-Phen}}$	$\omega_{T_{CT-Phen}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$	$\omega_{S_{CT-Naph}}$ ($\phi = 88^\circ$)
14.98	18.18	15.65	15.53	21.48	21.65	18.32
17.49	22.85	23.15	21.50	23.26	23.80	22.81
21.40	31.93	30.94	22.80	27.57	27.01	31.09
38.50	38.20	34.67	33.20	38.86	39.18	38.10
46.64	39.66	45.53	45.15	44.43	44.20	39.38
48.04	49.43	51.49	49.70	48.33	47.93	49.32
56.31	55.32	54.47	54.31	61.27	61.20	54.68
60.00	68.55	64.22	59.62	63.29	63.00	68.13
71.09	88.62	89.92	86.07	85.76	85.72	88.73
95.46	95.63	105.29	110.17	93.19	93.42	95.48
137.90	127.26	126.58	115.43	131.61	131.56	127.38
140.14	136.99	139.97	139.79	140.95	140.28	136.81
159.31	161.44	161.55	153.23	154.52	154.36	161.42
166.49	169.01	173.61	175.21	172.25	172.22	168.95
178.95	178.72	177.06	177.82	177.37	176.90	178.64
204.05	205.27	210.08	196.91	202.15	202.13	205.28
229.79	223.34	213.75	210.80	227.50	227.85	222.70
248.69	241.50	257.74	232.40	230.33	230.55	241.54
258.66	270.17	268.53	258.45	253.19	253.49	270.08
284.55	286.54	279.71	261.56	282.10	282.30	286.44
292.66	293.34	295.36	292.23	285.40	285.66	293.18
295.08	297.10	301.41	297.91	295.87	295.50	296.91
336.82	316.68	317.16	318.82	316.93	316.69	316.50
372.52	368.34	373.08	366.82	364.82	364.62	368.20
389.67	388.89	384.01	385.39	382.99	382.91	388.73
417.23	409.20	415.64	391.93	393.44	393.50	409.07
417.49	414.52	417.11	415.23	416.70	416.63	414.46
426.30	415.10	417.53	416.07	417.10	417.05	415.08
436.47	422.21	425.52	425.82	422.61	422.80	422.22
453.76	458.32	438.35	439.76	452.09	452.18	458.28
458.70	464.86	444.55	447.88	456.23	456.33	464.31
478.44	482.81	469.63	455.81	460.65	460.97	482.59
482.30	482.97	479.85	479.90	475.60	475.52	482.87
483.10	503.48	483.01	481.20	481.19	481.38	503.34
489.15	517.60	490.04	492.66	485.68	485.65	517.55

molecule-1						
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 90.2°$)	$\omega_{S_{CT-Phen}}$	$\omega_{T_{CT-Phen}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$	$\omega_{S_{CT-Naph}}$ ($\phi = 88°$)
522.05	520.20	503.94	502.01	505.84	505.75	520.19
525.23	522.03	523.25	526.22	510.77	510.85	521.97
542.69	524.16	529.62	530.60	519.91	519.90	524.19
551.47	542.85	543.68	544.61	532.59	532.41	542.77
556.67	579.20	570.66	552.34	542.85	542.78	579.06
601.68	582.45	572.28	564.62	564.64	564.59	582.48
621.26	612.67	594.89	595.76	605.88	605.84	612.55
623.59	615.19	607.38	609.27	609.32	609.27	615.19
627.41	626.46	621.27	614.32	624.55	624.45	626.34
630.40	630.77	622.77	622.59	628.56	628.53	630.68
637.92	635.36	631.25	625.66	633.88	633.84	635.24
640.51	639.78	635.29	629.10	640.08	639.99	639.72
666.74	649.56	654.73	636.11	642.00	641.99	649.58
675.41	664.09	657.74	650.85	664.68	664.69	664.04
689.67	680.70	664.20	668.17	673.65	673.64	680.65
702.19	685.77	688.26	670.81	680.93	681.49	686.01
713.06	710.08	693.90	686.70	706.66	706.80	709.97
713.13	710.34	694.09	702.48	712.32	712.57	710.32
720.68	718.74	714.41	703.90	712.77	712.75	718.77
728.04	721.51	716.18	709.79	714.13	714.25	721.33
745.29	725.03	737.57	714.50	723.80	723.70	724.98
751.71	740.17	748.43	733.15	728.27	728.30	740.00
775.15	747.03	754.67	750.15	740.29	740.57	746.99
777.08	752.89	757.89	755.70	745.36	745.38	752.99
793.64	757.22	783.67	773.22	760.48	760.75	757.47
794.69	778.10	788.40	788.45	774.07	774.08	778.06
806.03	780.42	790.88	791.11	777.78	777.83	780.39
819.29	787.32	794.73	796.22	786.89	786.91	787.29
827.52	798.44	804.74	804.90	797.64	797.70	798.44
828.89	813.39	813.02	814.61	820.04	820.56	813.39
858.22	837.57	829.76	816.44	830.55	830.34	837.76
858.69	843.51	831.07	834.01	831.50	831.43	843.48
870.22	844.67	863.63	852.05	855.73	855.94	844.43
879.16	858.49	869.91	852.88	858.45	858.75	858.31
882.02	858.75	874.78	855.83	858.52	858.83	858.68
882.60	861.77	876.07	874.84	861.68	861.72	861.72
917.90	891.64	893.65	886.72	879.80	880.24	891.26
933.47	893.43	894.47	900.98	882.89	883.17	893.09
933.99	904.27	901.18	924.66	904.45	904.47	904.51
936.24	913.68	930.65	929.96	913.65	913.69	913.59

molecule-1						
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 90.2^\circ$)	$\omega_{S_{CT-Phen}}$	$\omega_{T_{CT-Phen}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$	$\omega_{S_{CT-Naph}}$ ($\phi = 88^\circ$)
943.77	916.98	932.11	932.49	931.37	930.96	917.05
950.88	928.36	939.20	938.71	935.66	935.67	928.39
950.99	944.31	949.37	946.36	937.62	937.87	944.18
960.18	945.63	949.86	961.39	938.13	938.40	945.49
980.42	958.84	976.36	964.39	950.03	949.81	958.74
989.13	987.39	976.52	964.98	953.71	953.75	987.51
989.46	988.51	977.88	976.74	959.87	959.54	988.28
1000.8	994.12	988.96	979.03	961.26	960.50	994.00
1008.21	994.41	989.09	988.86	990.28	990.42	994.40
1008.29	1013.42	990.52	990.26	990.55	990.75	1013.36
1010.69	1013.64	996.51	1001.57	1004.86	1004.55	1013.58
1012.31	1016.03	1000.57	1007.34	1009.92	1010.02	1015.99
1012.71	1016.06	1009.60	1010.55	1010.28	1010.40	1016.01
1036.92	1021.05	1019.71	1011.30	1012.66	1012.69	1021.05
1041.04	1038.73	1022.69	1029.14	1013.02	1013.04	1038.57
1044.81	1041.24	1041.12	1036.38	1040.33	1040.34	1041.03
1059.70	1052.72	1041.38	1038.45	1044.68	1044.68	1052.73
1067.51	1061.26	1044.72	1055.99	1057.32	1057.23	1061.06
1067.92	1062.43	1061.97	1060.65	1065.59	1065.65	1062.24
1096.56	1076.27	1093.12	1092.20	1067.69	1067.66	1076.27
1101.93	1100.28	1104.27	1097.10	1068.72	1068.93	1100.38
1102.21	1106.70	1104.63	1103.93	1102.88	1102.75	1106.59
1136.04	1107.08	1155.14	1141.39	1103.06	1103.13	1107.02
1158.45	1150.04	1165.97	1149.65	1138.61	1138.58	1150.20
1167.58	1154.70	1171.84	1164.28	1139.91	1140.03	1154.94
1176.51	1162.44	1172.06	1168.83	1150.42	1150.55	1162.50
1176.80	1173.23	1174.23	1170.77	1165.80	1165.47	1173.26
1176.92	1179.90	1174.62	1176.81	1177.02	1176.98	1179.94
1188.41	1180.54	1181.21	1180.51	1177.68	1177.86	1180.36
1190.74	1196.10	1186.64	1184.99	1192.53	1192.72	1196.12
1200.90	1200.48	1195.07	1193.68	1197.02	1196.95	1200.45
1202.42	1204.83	1210.43	1202.02	1201.30	1201.25	1204.74
1212.92	1206.27	1212.69	1209.70	1202.82	1202.91	1206.17
1231.32	1207.65	1227.73	1231.25	1204.61	1204.60	1207.42
1241.30	1224.59	1237.64	1237.82	1219.35	1219.43	1224.53
1256.96	1255.86	1243.86	1245.58	1254.47	1254.68	1255.33
1277.88	1270.65	1281.83	1258.08	1264.07	1263.93	1270.39
1283.90	1285.67	1282.43	1279.49	1271.62	1271.85	1285.64

molecule-1						
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 90.2°$)	$\omega_{S_{CT-Phen}}$	$\omega_{T_{CT-Phen}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$	$\omega_{S_{CT-Naph}}$ ($\phi = 88°$)
1290.63	1292.38	1287.35	1286.42	1286.68	1286.85	1292.30
1302.25	1300.18	1303.96	1295.20	1294.50	1294.38	1300.09
1313.13	1302.85	1318.68	1315.94	1302.73	1302.68	1302.85
1315.53	1316.81	1328.93	1322.79	1311.84	1312.07	1316.72
1324.04	1326.63	1332.80	1333.60	1317.97	1318.01	1326.63
1333.25	1329.48	1339.01	1341.65	1321.60	1321.60	1329.44
1339.28	1351.19	1353.57	1348.83	1325.24	1325.33	1351.16
1351.91	1353.06	1354.92	1357.64	1331.19	1331.30	1352.92
1361.19	1358.01	1373.40	1371.10	1340.19	1340.25	1358.14
1361.26	1359.33	1375.77	1374.10	1345.24	1345.17	1359.33
1367.61	1367.13	1380.98	1387.68	1358.15	1358.01	1367.18
1390.89	1371.85	1414.76	1391.33	1360.98	1360.91	1371.85
1419.67	1391.11	1426.17	1398.55	1411.43	1411.20	1391.06
1431.74	1425.18	1435.59	1420.50	1428.18	1428.28	1425.24
1454.29	1441.98	1446.64	1448.67	1432.31	1432.33	1441.91
1468.01	1447.11	1459.62	1462.26	1437.48	1437.52	1447.24
1477.64	1461.19	1478.07	1469.55	1453.80	1453.89	1461.17
1484.12	1468.94	1486.49	1471.77	1464.38	1464.64	1468.81
1495.18	1475.81	1488.41	1482.30	1472.25	1472.00	1475.74
1510.94	1480.40	1492.52	1490.18	1477.89	1477.92	1480.37
1521.06	1492.15	1498.40	1494.85	1485.76	1485.80	1492.11
1536.81	1515.16	1503.75	1505.48	1504.69	1504.81	1515.13
1542.02	1529.99	1513.75	1530.32	1515.88	1515.92	1529.95
1551.52	1532.85	1519.77	1534.92	1525.85	1525.98	1532.90
1582.13	1536.87	1532.00	1540.95	1533.32	1533.33	1536.84
1609.65	1539.23	1542.84	1543.08	1541.24	1541.27	1539.23
1610.55	1554.08	1573.88	1556.41	1563.68	1563.76	1554.02
1614.94	1597.79	1574.38	1592.03	1576.21	1576.18	1597.72
1628.81	1599.42	1592.97	1596.93	1608.49	1608.50	1599.44
1628.99	1613.20	1611.71	1609.35	1615.34	1615.32	1613.15
1635.69	1616.87	1629.92	1610.15	1623.34	1623.43	1616.84
1638.09	1617.91	1632.51	1634.32	1624.28	1624.30	1617.89
1640.41	1635.67	1639.57	1637.16	1637.47	1637.53	1635.65
1661.51	1638.62	1654.66	1651.32	1639.47	1639.47	1638.60
1668.33	1658.05	1830.03	1662.10	1659.89	1659.97	1658.00
3162.35	3140.82	3157.95	3154.86	3163.40	3163.54	3140.89
3162.39	3149.38	3158.41	3159.15	3163.82	3163.96	3149.42
3166.68	3152.15	3163.22	3163.76	3164.28	3164.21	3152.17
3167.78	3164.05	3163.35	3169.38	3169.40	3169.59	3164.11
3167.97	3165.26	3169.74	3169.49	3169.91	3169.83	3165.33

molecule-1						
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 90.2^\circ$)	$\omega_{S_{CT-Phen}}$	$\omega_{T_{CT-Phen}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$	$\omega_{S_{CT-Naph}}$ ($\phi = 88^\circ$)
3170.24	3169.59	3174.32	3173.89	3169.99	3170.23	3169.58
3175.57	3169.67	3177.90	3178.10	3171.98	3172.14	3169.60
3176.84	3175.68	3180.17	3179.28	3178.12	3178.36	3175.54
3177.08	3175.68	3180.88	3183.91	3178.65	3178.52	3175.70
3181.52	3178.02	3184.78	3183.91	3181.30	3181.45	3178.06
3181.75	3183.27	3185.34	3188.39	3183.34	3183.45	3183.13
3183.24	3183.28	3189.79	3189.97	3183.79	3183.67	3183.29
3185.71	3184.61	3190.33	3190.59	3184.88	3185.03	3184.68
3185.92	3189.26	3190.67	3191.54	3189.94	3189.90	3189.13
3188.30	3189.33	3191.06	3194.02	3190.35	3190.04	3189.36
3190.59	3196.47	3199.03	3194.29	3192.34	3192.53	3196.45
3190.66	3196.55	3200.68	3197.86	3192.64	3192.56	3196.50
3192.26	3203.96	3200.94	3199.71	3193.97	3194.22	3203.98
3192.55	3204.31	3201.47	3200.19	3195.45	3195.78	3204.35
3195.54	3209.72	3203.52	3200.54	3196.34	3196.13	3209.48
3199.53	3210.15	3204.19	3211.48	3198.03	3198.10	3210.02
3206.06	3230.51	3214.19	3212.66	3211.96	3211.99	3230.40
3206.50	3231.07	3214.95	3223.46	3222.43	3222.30	3230.95

molecule-1						
$\omega_{S_{CT-Naph}}$ ($\phi = 84^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 80^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 76^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 72^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 68^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 64^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 60^\circ$)
19.45	19.74	20.41	22.59	23.41	22.57	20.68
22.39	22.34	23.22	24.75	26.84	26.97	24.55
30.14	30.52	31.56	32.34	33.34	33.31	32.46
37.92	38.16	38.91	40.66	42.05	42.21	42.23
40.73	41.59	43.04	45.22	47.54	48.82	49.20
49.23	49.42	49.55	49.99	50.24	50.29	50.47
55.37	55.92	57.88	61.50	63.71	66.83	69.88
67.30	67.50	68.73	70.33	71.60	71.87	72.00
89.09	89.75	91.48	93.16	94.35	94.72	94.42
95.40	95.67	96.00	97.08	98.87	100.77	102.32
128.12	128.63	129.63	131.98	134.70	136.90	137.58
136.78	137.32	139.41	141.76	144.81	147.58	149.66
161.80	162.43	164.14	166.32	168.16	169.25	169.75

molecule-1						
$\omega_{S_{CT-Naph}}$ ($\phi = 84^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 80^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 76^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 72^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 68^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 64^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 60^\circ$)
169.17	169.55	170.54	172.69	177.44	184.36	190.75
179.36	180.51	182.53	187.90	195.15	204.92	209.13
205.31	205.38	205.61	206.13	206.87	208.38	217.35
223.38	223.47	223.82	225.42	224.83	224.04	226.77
241.61	240.94	240.56	240.75	241.23	242.12	242.36
270.10	270.25	270.43	270.66	270.72	270.55	270.36
286.56	286.61	286.86	288.26	289.29	290.72	292.10
293.40	293.06	292.70	293.00	292.97	293.17	293.49
296.70	296.71	297.07	297.73	298.23	298.61	299.01
316.64	316.57	317.04	318.17	319.23	321.20	323.61
368.29	368.04	368.18	369.17	370.11	371.45	373.96
388.52	388.28	388.23	388.38	388.62	389.42	390.21
408.70	407.96	407.43	406.90	406.43	406.16	405.96
414.53	414.54	414.64	414.80	414.96	414.58	414.62
414.73	414.64	414.79	415.13	415.11	414.89	414.79
422.28	422.62	423.09	423.66	424.49	425.46	426.27
458.23	458.15	458.64	459.02	459.34	459.81	460.63
464.62	464.53	465.19	466.37	466.56	468.34	471.27
482.72	482.82	483.01	483.52	483.83	483.94	484.08
482.88	482.99	483.51	484.34	485.14	486.64	490.40
502.75	501.88	500.76	499.75	499.01	498.73	498.71
517.46	517.38	517.35	517.39	517.42	517.33	517.25
520.55	520.63	520.67	521.16	521.70	522.63	523.83
521.87	521.84	522.41	523.42	523.87	524.04	524.04
524.18	524.14	524.23	524.55	525.78	527.68	529.94
542.69	542.78	542.87	543.17	543.33	543.34	543.34
578.36	577.25	575.86	574.25	572.52	570.93	569.08
582.78	583.15	583.77	584.68	585.64	586.74	587.92
612.25	611.78	611.23	610.87	610.52	610.29	609.95
615.15	615.06	615.10	615.13	615.14	615.18	615.26
626.42	626.25	626.05	625.93	625.51	625.27	625.51
630.65	630.73	630.80	630.90	630.93	630.88	630.83
635.10	634.80	634.53	634.36	634.18	634.22	634.50
639.75	639.67	639.59	639.55	639.45	639.48	639.69
649.48	649.21	649.07	648.83	648.40	648.10	647.84
664.01	664.05	664.14	664.31	664.44	664.54	664.64

molecule-1						
$\omega_{S_{CT-Naph}}$ ($\phi = 84^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 80^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 76^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 72^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 68^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 64^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 60^\circ$)
680.62	680.52	680.46	680.46	680.33	680.25	680.16
686.88	687.48	687.87	689.66	692.18	696.11	700.32
709.89	709.88	709.99	710.18	710.21	709.74	709.62
709.99	709.97	710.04	710.27	710.39	710.25	710.16
719.12	719.05	718.95	718.35	717.19	716.35	716.20
721.60	721.60	721.49	722.91	724.21	724.78	724.90
724.95	725.01	725.14	725.48	726.50	729.47	733.16
739.74	739.53	739.58	739.28	738.50	738.22	738.22
746.94	746.84	746.76	746.65	746.47	746.31	746.10
753.46	754.14	754.88	756.01	757.83	760.73	764.31
758.66	759.64	760.90	764.35	768.88	775.03	776.64
778.02	777.87	777.71	777.65	777.51	777.42	779.31
780.31	780.19	780.08	779.93	779.74	779.52	781.98
787.28	787.25	787.32	787.57	787.83	788.33	789.18
798.47	798.44	798.50	798.61	798.74	798.97	799.19
813.73	813.84	814.18	815.72	817.93	820.95	823.87
838.39	838.86	839.47	839.62	838.62	837.59	836.75
843.12	841.81	841.35	841.01	841.80	843.27	845.21
843.98	843.33	843.09	842.62	844.07	847.70	852.09
858.01	857.95	858.12	858.38	858.50	857.85	857.51
858.30	858.32	858.46	858.64	858.65	858.59	858.48
861.81	862.00	862.37	863.05	863.68	864.41	865.13
890.30	889.58	889.08	888.46	886.28	883.12	879.29
892.18	891.37	890.90	890.49	890.38	889.22	888.36
905.12	905.55	906.05	907.37	908.79	909.70	910.04
913.15	912.63	912.25	912.27	912.88	915.03	918.75
917.55	918.31	919.19	920.09	920.90	921.59	922.13
928.74	929.31	930.14	931.24	932.29	933.44	934.82
943.86	943.70	943.70	943.84	943.89	943.32	942.82
945.13	945.09	945.17	945.31	945.12	944.43	943.97
958.66	958.80	958.97	959.13	959.21	959.25	959.19
987.08	985.20	984.03	981.99	980.38	978.53	976.55
987.70	987.09	986.63	985.64	984.88	985.59	986.67
993.77	993.69	993.79	993.89	993.79	993.24	992.96
994.10	993.99	993.99	994.01	993.97	993.82	993.65
1013.31	1013.39	1013.42	1013.46	1013.49	1013.44	1013.33
1013.53	1013.61	1013.63	1013.68	1013.68	1013.62	1013.55
1015.87	1015.77	1015.71	1015.60	1015.24	1014.74	1014.34

molecule-1						
$\omega_{S_{CT-Naph}}$ ($\phi = 84^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 80^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 76^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 72^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 68^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 64^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 60^\circ$)
1015.89	1015.88	1015.79	1015.64	1015.54	1015.31	1015.08
1021.33	1021.60	1021.98	1022.63	1023.39	1024.24	1025.02
1038.48	1038.85	1039.22	1039.65	1039.98	1040.26	1040.58
1040.90	1041.38	1041.87	1042.44	1042.91	1043.31	1043.72
1053.14	1053.61	1054.15	1055.05	1056.10	1057.34	1058.43
1060.92	1061.27	1061.72	1062.20	1062.66	1062.98	1063.29
1062.16	1062.51	1062.95	1063.46	1064.04	1064.57	1065.21
1076.84	1077.27	1077.44	1078.63	1080.16	1082.45	1084.73
1100.66	1100.91	1101.21	1101.95	1103.18	1104.87	1106.27
1106.43	1106.41	1106.37	1106.66	1106.96	1106.68	1106.50
1106.66	1106.65	1106.83	1107.04	1107.22	1107.30	1107.04
1150.58	1151.03	1151.87	1153.09	1154.43	1156.14	1158.21
1155.51	1155.89	1156.29	1157.14	1158.05	1159.51	1161.23
1162.65	1162.72	1162.80	1163.08	1163.53	1164.36	1165.49
1173.74	1174.16	1174.60	1175.68	1176.86	1178.67	1179.24
1179.96	1179.85	1179.71	1179.68	1179.69	1179.74	1179.66
1180.10	1179.99	1179.85	1179.77	1179.84	1179.94	1181.17
1196.68	1197.15	1197.75	1199.03	1200.12	1201.10	1201.70
1200.62	1201.15	1201.90	1202.95	1204.10	1204.69	1204.31
1204.50	1204.61	1205.01	1205.71	1206.32	1206.67	1207.09
1206.06	1206.18	1206.58	1207.30	1208.35	1209.95	1212.61
1207.41	1208.13	1208.87	1210.19	1211.29	1212.75	1214.51
1224.65	1225.04	1225.41	1225.94	1226.61	1227.55	1228.54
1254.84	1255.80	1256.70	1257.63	1258.17	1258.55	1258.84
1271.06	1270.99	1270.69	1272.05	1273.46	1275.86	1278.02
1285.71	1285.99	1286.45	1287.22	1288.19	1289.38	1290.87
1292.43	1293.07	1293.95	1295.05	1295.86	1296.48	1296.76
1300.15	1300.30	1300.54	1301.15	1301.66	1302.37	1303.90
1302.85	1302.99	1303.25	1303.69	1304.13	1304.63	1305.24
1316.62	1316.66	1316.59	1316.44	1316.05	1315.49	1314.77
1326.67	1326.72	1326.82	1327.02	1327.22	1327.51	1327.90
1329.50	1329.60	1329.70	1329.85	1329.91	1330.01	1330.27
1351.23	1351.55	1351.65	1351.64	1351.51	1351.15	1350.64
1352.44	1352.07	1352.30	1352.90	1353.50	1353.78	1353.95
1358.80	1358.78	1358.50	1358.29	1358.22	1358.16	1357.99
1359.55	1360.65	1361.93	1362.98	1363.70	1364.14	1364.51
1367.52	1368.51	1370.25	1372.70	1375.23	1377.47	1379.37

molecule-1						
$\omega_{S_{CT-Naph}}$ ($\phi = 84^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 80^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 76^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 72^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 68^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 64^\circ$)	$\omega_{S_{CT-Naph}}$ ($\phi = 60^\circ$)
1372.11	1372.90	1374.10	1375.69	1377.82	1380.71	1383.72
1390.94	1390.83	1390.64	1390.37	1390.17	1390.12	1390.36
1425.61	1426.03	1426.55	1427.49	1428.76	1430.30	1431.51
1441.91	1442.06	1442.27	1442.67	1443.06	1443.53	1444.17
1447.56	1447.82	1448.16	1448.70	1449.38	1450.46	1451.84
1461.23	1461.25	1461.29	1461.40	1461.43	1461.51	1461.63
1469.46	1469.67	1469.72	1471.25	1473.05	1475.84	1477.98
1475.81	1476.18	1476.66	1477.25	1477.76	1478.20	1479.21
1480.37	1480.39	1480.48	1480.79	1481.24	1482.01	1483.44
1492.09	1492.05	1492.03	1492.09	1492.02	1491.89	1491.77
1515.19	1515.35	1515.61	1516.02	1516.41	1516.75	1517.24
1529.84	1529.84	1529.88	1529.98	1530.02	1529.88	1529.60
1533.42	1534.15	1535.05	1536.29	1537.28	1537.47	1537.64
1536.79	1536.89	1537.04	1537.27	1537.88	1539.10	1539.58
1539.39	1539.52	1539.61	1539.92	1540.32	1541.33	1542.98
1553.70	1553.18	1552.53	1551.83	1550.98	1550.23	1549.78
1597.47	1597.10	1596.55	1595.84	1594.96	1594.10	1593.28
1599.37	1599.17	1598.95	1598.79	1598.60	1598.37	1598.00
1613.04	1612.93	1612.70	1612.39	1611.88	1611.17	1610.28
1616.80	1616.71	1616.59	1616.48	1616.38	1616.16	1615.85
1617.78	1617.56	1617.24	1616.92	1616.61	1616.35	1616.13
1635.61	1635.59	1635.57	1635.52	1635.43	1635.25	1634.99
1638.56	1638.51	1638.47	1638.40	1638.33	1638.18	1637.96
1657.87	1657.63	1657.33	1657.05	1656.60	1656.10	1655.71
3141.00	3141.07	3141.19	3141.47	3141.87	3142.26	3142.56
3149.54	3149.72	3150.00	3150.37	3150.90	3151.45	3151.99
3152.23	3152.31	3152.53	3152.79	3153.19	3153.61	3153.95
3164.23	3164.35	3164.56	3164.91	3165.40	3165.89	3166.35
3165.42	3165.54	3165.87	3166.24	3166.84	3167.41	3167.79
3169.53	3169.60	3169.60	3169.58	3169.53	3169.41	3169.25
3169.56	3169.61	3169.61	3169.62	3169.54	3169.47	3169.46
3175.47	3175.49	3175.50	3175.62	3175.58	3175.53	3175.47
3175.62	3175.86	3175.95	3175.96	3175.92	3175.70	3175.56
3178.07	3178.14	3178.47	3178.84	3179.51	3180.11	3180.29

molecule-1						
$\omega_{S_{CT-Naph}}$ ($\phi = 84^{\circ}$)	$\omega_{S_{CT-Naph}}$ ($\phi = 80^{\circ}$)	$\omega_{S_{CT-Naph}}$ ($\phi = 76^{\circ}$)	$\omega_{S_{CT-Naph}}$ ($\phi = 72^{\circ}$)	$\omega_{S_{CT-Naph}}$ ($\phi = 68^{\circ}$)	$\omega_{S_{CT-Naph}}$ ($\phi = 64^{\circ}$)	$\omega_{S_{CT-Naph}}$ ($\phi = 60^{\circ}$)
3183.05	3183.06	3183.02	3183.19	3183.24	3183.22	3183.09
3183.16	3183.48	3183.61	3183.64	3183.61	3183.35	3183.24
3184.82	3184.77	3184.80	3185.03	3185.27	3185.47	3185.46
3189.11	3189.10	3189.06	3189.18	3189.23	3189.22	3189.21
3189.24	3189.46	3189.56	3189.60	3189.62	3189.42	3189.22
3196.41	3196.46	3196.44	3196.46	3196.47	3196.44	3196.34
3196.47	3196.51	3196.50	3196.52	3196.54	3196.49	3196.45
3203.71	3203.63	3203.60	3203.39	3203.32	3203.09	3202.59
3204.27	3203.98	3203.83	3203.91	3203.87	3203.67	3203.15
3209.12	3209.15	3209.34	3209.34	3209.36	3209.15	3208.57
3209.72	3209.58	3209.69	3209.76	3209.73	3209.73	3209.83
3230.26	3230.34	3230.45	3230.09	3229.28	3228.19	3226.19
3230.79	3230.99	3231.47	3231.56	3232.17	3232.76	3232.21

S14 Frequencies of all geometries of molecule 2 computed at (B3LYP/6-311G(d,p)) level of theory

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
10.52	12.76	12.76	12.13	13.27	13.20
16.48	16.17	16.17	14.98	18.09	18.13
17.12	18.43	18.43	19.85	18.71	18.49
18.41	22.24	22.25	22.21	19.40	19.36
23.43	22.95	22.94	23.96	27.01	26.97
28.16	27.99	27.99	27.82	28.38	28.12
41.01	36.87	36.86	39.99	41.90	41.82
42.62	48.43	48.43	45.23	49.03	49.04
45.47	50.55	50.54	53.34	49.65	49.66
51.55	56.92	56.91	56.81	51.89	51.83
73.52	72.91	72.91	67.19	73.46	73.49
78.59	78.92	78.92	73.53	78.76	78.79
78.95	84.49	84.49	79.52	82.47	82.50
85.77	85.94	85.94	89.25	89.08	89.14
104.73	109.46	109.46	107.16	109.14	109.15
121.25	118.26	118.25	124.62	119.09	119.12
130.96	127.39	127.39	130.05	127.11	127.09
133.23	132.01	132.01	135.66	131.38	131.40
145.04	142.92	142.92	137.09	145.79	145.81
162.61	162.09	162.08	167.21	161.53	161.55
178.52	177.87	177.89	175.53	174.29	174.21
187.72	190.19	190.19	178.10	191.55	191.52
202.61	197.14	197.14	204.01	195.57	195.56
215.24	213.79	213.80	213.98	215.46	215.44
229.44	234.52	234.52	226.19	231.56	231.56
260.13	257.58	257.59	256.24	247.78	247.72
274.83	274.21	274.19	261.66	261.19	261.15
289.28	279.18	279.16	281.64	278.73	278.75
299.57	297.29	297.30	294.22	297.35	297.33

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
316.98	321.26	321.26	306.94	316.99	317.01
339.92	338.57	338.57	321.56	337.93	337.92
345.25	346.52	346.52	346.67	343.34	343.36
357.34	362.89	362.89	356.50	354.27	354.25
385.74	371.81	371.81	376.94	365.18	365.20
400.99	388.78	388.77	393.17	385.99	386.01
411.78	403.14	403.14	405.73	403.52	403.54
415.81	414.34	414.35	415.92	415.34	415.41
416.57	414.88	414.88	416.72	415.59	415.64
422.51	419.82	419.82	421.00	417.70	417.71
423.32	420.91	420.91	421.47	421.75	421.80
429.83	422.80	422.80	424.39	422.96	423.11
442.11	430.52	430.52	424.79	427.46	427.46
454.56	454.99	454.98	441.28	452.17	452.10
456.82	462.00	462.00	447.51	457.51	457.42
463.29	468.58	468.57	454.96	463.78	463.73
482.74	500.86	500.86	472.06	465.58	465.56
483.27	503.63	503.62	480.53	480.59	480.51
497.50	504.91	504.91	495.93	492.53	492.52
507.71	511.74	511.75	501.80	498.82	498.80
515.36	520.61	520.61	512.23	510.27	510.18
526.31	525.04	525.05	526.24	513.61	513.58
534.52	526.89	526.89	528.32	519.03	518.98
550.89	542.10	542.10	534.25	531.32	531.28
562.75	564.41	564.41	554.38	536.74	536.72
568.49	568.83	568.84	559.66	566.02	566.01
571.07	581.78	581.77	568.75	570.11	570.10
601.91	583.39	583.39	573.50	570.89	570.88
622.93	613.21	613.21	596.66	606.24	606.25
624.66	615.42	615.42	613.96	609.73	609.72
627.65	628.07	628.07	620.40	625.69	625.70
631.21	631.31	631.31	625.48	630.85	630.84
632.63	632.97	632.97	628.22	632.20	632.21
634.44	634.75	634.74	631.63	635.20	635.20
653.37	643.81	643.81	639.03	636.32	636.30
656.14	651.74	651.74	643.05	651.87	651.86
656.71	655.59	655.59	649.26	655.79	655.79

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
672.04	657.45	657.45	655.72	657.05	657.06
689.36	679.71	679.71	668.04	673.45	673.44
699.00	685.06	685.04	682.28	681.26	681.24
701.68	694.43	694.43	689.97	697.07	697.05
713.66	712.91	712.91	703.82	705.94	705.88
713.96	713.27	713.27	709.08	713.57	713.58
719.49	717.99	717.99	710.94	713.77	713.80
730.60	720.50	720.50	713.58	714.44	714.37
748.78	729.85	729.85	716.62	724.13	724.12
749.21	739.45	739.45	746.36	731.34	731.32
751.66	749.72	749.72	747.28	740.24	740.18
765.70	750.28	750.28	750.84	748.66	748.66
776.10	753.04	753.00	751.77	749.42	749.42
783.05	757.65	757.63	766.45	759.22	759.29
783.43	764.32	764.33	772.01	763.00	763.01
793.64	775.81	775.81	782.57	776.55	776.52
796.73	783.67	783.67	784.50	782.85	782.85
806.83	784.39	784.39	789.57	783.62	783.63
819.27	791.48	791.48	795.51	791.32	791.29
824.15	798.64	798.64	805.45	797.95	797.94
825.55	813.22	813.21	810.88	820.22	820.16
852.12	837.34	837.34	817.26	826.96	826.81
852.36	838.34	838.35	818.14	828.38	828.23
859.40	839.33	839.34	830.42	852.24	852.32
859.59	851.25	851.26	845.21	852.45	852.50
859.82	852.05	852.06	849.95	855.80	855.83
860.24	859.07	859.08	858.25	858.70	858.74
872.38	859.82	859.82	859.65	859.52	859.63
881.64	861.06	861.06	861.40	859.81	859.90
884.48	864.76	864.76	877.34	860.96	860.92
887.78	867.79	867.80	890.84	865.65	865.58
918.40	894.12	894.12	904.70	884.89	884.85
934.53	896.17	896.17	912.07	889.28	889.22
937.48	903.60	903.61	927.48	905.04	905.03
937.76	914.05	914.05	934.56	914.11	914.11
943.99	917.03	917.04	938.03	931.14	931.29

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
950.17	927.90	927.90	941.88	937.23	937.05
950.50	940.28	940.28	951.97	938.04	938.19
960.26	940.64	940.64	958.57	938.17	938.34
980.38	958.13	958.13	963.72	949.91	950.11
981.20	984.62	984.62	964.33	953.93	953.92
981.37	984.90	984.90	973.75	959.41	959.45
988.70	988.30	988.30	980.34	960.38	960.40
989.46	989.19	989.19	982.01	982.16	982.35
990.76	991.48	991.48	982.43	982.55	982.66
990.96	991.54	991.54	989.74	989.29	989.57
1000.86	993.85	993.85	991.23	989.86	990.11
1009.79	994.01	994.01	991.97	990.96	991.21
1009.89	1011.77	1011.77	997.06	991.42	991.65
1010.70	1012.01	1012.01	1001.16	1004.98	1004.79
1011.21	1012.02	1012.02	1002.30	1010.07	1010.30
1011.45	1012.13	1012.13	1010.00	1010.14	1010.37
1020.08	1020.13	1020.13	1011.03	1011.44	1011.37
1020.22	1020.25	1020.25	1012.01	1011.76	1011.68
1034.41	1021.05	1021.05	1018.48	1020.22	1020.21
1037.03	1032.89	1032.90	1020.20	1020.30	1020.29
1037.12	1035.02	1035.02	1033.76	1034.33	1034.29
1054.59	1050.51	1050.51	1037.02	1037.13	1037.10
1057.65	1053.66	1053.66	1049.54	1053.26	1053.22
1061.38	1055.69	1055.69	1052.40	1057.68	1057.62
1069.65	1065.46	1065.46	1060.10	1060.06	1060.00
1070.19	1066.25	1066.25	1065.54	1066.57	1066.46
1096.65	1076.07	1076.05	1093.98	1070.02	1069.97
1102.20	1099.82	1099.83	1102.68	1070.87	1070.84
1102.39	1103.44	1103.44	1102.74	1102.54	1102.56
1136.36	1103.78	1103.78	1131.38	1102.84	1102.84
1141.55	1146.19	1146.18	1144.23	1139.03	1138.97
1142.17	1146.93	1146.92	1146.88	1140.19	1140.14
1159.06	1150.70	1150.70	1162.88	1142.64	1142.69

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
1167.54	1154.34	1154.36	1165.30	1143.24	1143.33
1176.87	1161.99	1161.99	1169.43	1151.34	1151.28
1177.03	1173.18	1173.18	1173.68	1165.86	1165.78
1177.07	1178.00	1178.00	1177.29	1177.42	1177.37
1188.57	1178.09	1178.09	1180.61	1177.42	1177.38
1191.48	1195.91	1195.92	1188.72	1193.80	1193.74
1200.35	1201.28	1201.28	1200.67	1198.29	1198.21
1200.59	1201.77	1201.77	1200.90	1200.79	1200.75
1208.49	1202.61	1202.67	1205.82	1201.22	1201.18
1214.47	1207.22	1207.24	1214.84	1204.42	1204.39
1218.79	1215.54	1215.54	1218.95	1211.55	1211.59
1231.44	1218.92	1218.91	1233.52	1215.13	1215.21
1241.57	1224.59	1224.57	1242.02	1223.28	1223.28
1258.77	1256.92	1256.92	1249.01	1256.57	1256.56
1278.13	1270.17	1270.18	1271.51	1262.88	1262.89
1280.89	1286.42	1286.43	1279.29	1271.81	1271.83
1283.66	1287.27	1287.28	1281.44	1282.75	1282.70
1291.62	1290.36	1290.36	1284.37	1285.68	1285.61
1298.74	1295.99	1296.00	1290.86	1294.14	1294.06
1302.59	1303.66	1303.65	1301.86	1302.15	1302.08
1302.79	1304.20	1304.20	1303.92	1302.86	1302.79
1308.39	1306.70	1306.70	1309.49	1303.48	1303.43
1314.83	1309.04	1309.04	1319.79	1307.47	1307.43
1317.60	1318.75	1318.76	1324.21	1313.15	1313.11
1324.71	1324.97	1324.97	1325.90	1317.98	1317.90
1329.37	1327.84	1327.84	1336.11	1321.16	1321.12
1336.79	1341.35	1341.35	1345.12	1326.70	1326.62
1340.07	1342.13	1342.13	1356.05	1329.36	1329.32
1351.31	1357.72	1357.71	1357.29	1336.95	1336.98
1356.87	1357.85	1357.84	1361.29	1340.83	1340.85
1357.24	1358.38	1358.38	1369.55	1347.79	1347.80
1358.30	1358.86	1358.88	1373.56	1351.59	1351.58
1367.57	1363.05	1363.05	1383.44	1357.22	1357.25
1390.82	1366.14	1366.13	1391.37	1357.65	1357.66
1419.59	1391.07	1391.03	1403.63	1411.50	1411.39

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
1423.19	1424.91	1424.91	1420.25	1422.92	1422.88
1430.10	1428.81	1428.82	1431.43	1429.52	1429.51
1444.99	1433.35	1433.35	1457.55	1429.88	1429.84
1464.79	1447.02	1447.02	1463.31	1436.99	1436.93
1468.22	1452.65	1452.67	1469.77	1445.72	1445.69
1477.21	1468.46	1468.46	1470.38	1464.17	1464.14
1479.69	1471.81	1471.82	1478.64	1465.86	1465.80
1494.96	1477.41	1477.40	1484.32	1472.64	1472.44
1512.42	1479.26	1479.25	1491.48	1477.44	1477.40
1518.26	1486.13	1486.14	1494.34	1480.54	1480.51
1525.13	1515.56	1515.56	1503.25	1506.57	1506.57
1537.62	1521.02	1521.02	1510.02	1516.31	1516.30
1542.25	1525.98	1525.97	1521.37	1522.36	1522.32
1552.35	1532.68	1532.67	1524.53	1523.83	1523.80
1558.16	1539.00	1538.99	1540.26	1532.54	1532.49
1573.83	1549.75	1549.74	1543.28	1551.12	1551.12
1584.75	1550.83	1550.82	1550.11	1552.31	1552.31
1595.30	1552.13	1552.12	1552.94	1563.74	1563.72
1610.57	1582.49	1582.48	1583.31	1569.60	1569.57
1616.10	1588.81	1588.81	1586.97	1584.78	1584.72
1616.72	1599.10	1599.12	1592.87	1593.58	1593.53
1627.36	1603.24	1603.22	1603.35	1615.83	1615.75
1627.82	1613.80	1613.81	1610.46	1617.00	1616.91
1635.78	1617.11	1617.11	1615.91	1621.52	1621.47
1637.63	1617.38	1617.38	1628.29	1622.08	1622.04
1638.56	1636.32	1636.32	1636.23	1637.53	1637.42
1644.90	1638.09	1638.09	1637.22	1638.39	1638.28
1647.49	1641.57	1641.57	1643.32	1643.99	1643.91
1661.65	1645.56	1645.56	1654.99	1646.94	1646.87
1668.58	1659.61	1659.62	1662.93	1660.71	1660.68
3162.94	3140.85	3140.86	3158.35	3163.31	3163.44
3163.03	3149.08	3149.11	3163.24	3163.36	3163.48
3166.77	3151.96	3151.98	3163.40	3163.38	3163.53
3167.75	3163.74	3163.77	3168.50	3168.46	3168.57

molecule-2					
ω_{S_0}	$\omega_{S_{CT-Naph}}$ ($\phi = 89.53^\circ$)	$\omega_{S_{CT-Biph}}$	$\omega_{T_{CT-Biph}}$	$\omega_{T_{CT-Naph}}$	$\omega_{T_{LE-Naph}}$
3167.80	3164.83	3164.85	3168.58	3168.51	3168.60
3169.70	3165.06	3165.06	3169.35	3170.19	3170.33
3169.92	3165.07	3165.07	3169.66	3171.34	3171.47
3170.32	3170.49	3170.49	3171.86	3171.51	3171.58
3171.24	3170.55	3170.55	3173.23	3172.07	3172.19
3171.44	3176.17	3176.17	3174.11	3172.66	3172.80
3175.63	3176.78	3176.77	3178.15	3172.93	3173.02
3177.92	3177.37	3177.39	3178.68	3178.38	3178.45
3177.99	3177.75	3177.75	3180.95	3178.44	3178.52
3182.22	3178.50	3178.49	3183.35	3181.44	3181.55
3182.27	3180.31	3180.31	3185.19	3183.11	3183.16
3183.45	3180.35	3180.35	3187.03	3183.11	3183.19
3184.40	3184.51	3184.51	3188.50	3185.04	3185.10
3185.81	3185.11	3185.11	3189.96	3186.46	3186.54
3185.86	3191.26	3191.26	3190.05	3188.02	3188.09
3188.28	3192.04	3192.04	3191.86	3188.03	3188.11
3188.42	3192.29	3192.29	3192.28	3191.26	3191.33
3188.51	3192.61	3192.60	3194.47	3191.85	3191.90
3191.79	3194.38	3194.38	3195.48	3192.33	3192.41
3191.81	3194.92	3194.92	3199.14	3192.75	3192.80
3192.63	3204.38	3204.36	3199.73	3194.38	3194.40
3192.92	3205.07	3205.05	3200.64	3196.59	3196.58
3195.77	3209.83	3209.83	3201.63	3197.21	3197.18
3199.54	3210.25	3210.25	3214.34	3197.82	3197.85
3206.36	3229.85	3229.84	3214.77	3213.27	3213.26
3206.80	3230.54	3230.54	3223.45	3221.85	3221.76

S15 Coordinates of the optimized geometries of molecule 1

S_0 geometry (Å) (B3LYP/6-311G(d,p))

C	-6.64994200	-0.67600800	0.82481800
C	-5.25268700	-0.52449500	0.86281200
C	-4.65766200	0.69524500	0.59948800
C	-5.42206300	1.82958600	0.27693000
C	-6.81072900	1.68179200	0.23958300
C	-7.41141100	0.45351300	0.50904800
C	-3.36841100	3.08908500	0.02090800
C	-2.64503000	1.92948600	0.34817200
C	-1.26270500	1.92218000	0.36383700
H	-0.76796200	0.98805100	0.59990300
C	-0.52518900	3.07981400	0.05952900
C	-1.24434000	4.23546900	-0.26072200
C	-2.63778800	4.24096600	-0.28087500
H	-4.60321200	-1.36350000	1.08046100
H	-7.42850300	2.53820600	0.00494100
H	-3.16450700	5.15331300	-0.52656300
H	-8.49258700	0.39129800	0.49292000
H	-0.71975600	5.15804400	-0.47704800
N	-4.77295800	3.04800600	0.01512700
O	-3.27746200	0.74144300	0.66409500
C	0.95823000	3.06762600	0.08438600
C	1.70235900	3.83059800	-0.83067900
C	1.66165000	2.29473300	1.02285600
C	3.09447500	3.82395000	-0.80546600
H	1.18716200	4.41704400	-1.58268100
C	3.05391200	2.28538500	1.04568900
H	1.11496600	1.71257400	1.75583400
C	3.77805900	3.05072300	0.13236300
H	3.64599600	4.41668300	-1.52679400
H	3.57339000	1.68536500	1.78455300
C	-7.28364900	-1.98605900	1.11387700
C	-8.44631900	-2.39075500	0.43736100
C	-6.74147000	-2.85898300	2.07145000
C	-9.04502000	-3.61776300	0.71046600
H	-8.87308000	-1.74906400	-0.32481300
C	-7.33832900	-4.08763800	2.34202500
H	-5.85725100	-2.56507700	2.62528700
C	-8.49396000	-4.47346500	1.66377900
H	-9.93845400	-3.90978100	0.16981100
H	-6.90391200	-4.74079000	3.09067500
C	-5.53109500	4.20667000	-0.36645900
C	-5.96780100	5.12389400	0.63593400
C	-5.82678600	4.41816300	-1.69332600
C	-5.68728000	4.94809200	2.01652500
C	-6.72177800	6.27015500	0.22308500
C	-6.57108300	5.55082900	-2.09228100
H	-5.48232600	3.70527900	-2.43320900
C	-6.13080500	5.86171700	2.94298000
H	-5.11790100	4.08296700	2.33212300
C	-7.16303200	7.19252900	1.20901500
C	-7.00776600	6.45491700	-1.15500800

H	-6.79331500	5.69874300	-3.14234800
C	-6.87530700	6.99453000	2.53763500
H	-5.90967500	5.71553700	3.99403400
H	-7.73326300	8.05916600	0.89246100
H	-7.57949900	7.32570000	-1.45687800
H	-7.21738900	7.70531500	3.28094000
H	-8.95898600	-5.42959900	1.87484300
H	4.86185400	3.04409800	0.15059200

$S_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-6.62510600	-0.66646100	0.81849300
C	-5.23412100	-0.54368400	0.84018500
C	-4.63543900	0.67225300	0.55244600
C	-5.39783700	1.81753000	0.22488300
C	-6.79907700	1.68965700	0.20537100
C	-7.39081300	0.47971300	0.49490000
C	-3.37598100	3.05771100	-0.02411900
C	-2.64168800	1.89469700	0.30513500
C	-1.25665400	1.89426200	0.34383400
H	-0.75551300	0.96392700	0.57537200
C	-0.54383000	3.06135500	0.06082100
C	-1.27681600	4.22863800	-0.26287000
C	-2.65377700	4.23219000	-0.30575700
H	-4.59207100	-1.38689900	1.05712100
H	-7.39425400	2.55902400	-0.03241900
H	-3.20192100	5.13095900	-0.54723000
H	-8.47089800	0.41622000	0.49608900
H	-0.74802000	5.15161100	-0.46078600
N	-4.75816500	3.00981700	-0.06400700
O	-3.27424600	0.72097400	0.58514200
C	0.93541000	3.07860200	0.10123300
C	1.66775700	3.88360000	-0.78672600
C	1.64047300	2.29053400	1.02569900
C	3.05872100	3.89515900	-0.75384300
H	1.14929500	4.48357000	-1.52500100
C	3.03102500	2.30839800	1.06096100
H	1.09868700	1.68082200	1.73898900
C	3.74576900	3.10927500	0.17057300
H	3.60618500	4.51453500	-1.45476400
H	3.55663900	1.70153700	1.78903400
C	-7.28028000	-1.95668000	1.12876300
C	-8.46956700	-2.33117800	0.48211900
C	-6.72824800	-2.83616500	2.07461800
C	-9.08240400	-3.54701100	0.76871000
H	-8.90411800	-1.68185800	-0.26839900
C	-7.34603600	-4.04847300	2.36419400
H	-5.82569000	-2.55931900	2.60634300
C	-8.52446400	-4.40957300	1.71150700
H	-9.99359200	-3.82294200	0.25081200
H	-6.91045300	-4.70865200	3.10519000
C	-5.52455800	4.18886800	-0.41699200
C	-5.93950200	5.06982600	0.62345800
C	-5.82081400	4.40545000	-1.78444500
C	-5.65780000	4.87673400	1.99558700

C	-6.70158500	6.23680800	0.22242700
C	-6.55026300	5.52843600	-2.13797800
H	-5.47632200	3.69710300	-2.52829900
C	-6.10304700	5.79378300	2.96654000
H	-5.08965700	4.00919600	2.30998500
C	-7.12854300	7.13182900	1.23181800
C	-6.98786900	6.43528000	-1.15887300
H	-6.78479500	5.70745300	-3.18203800
C	-6.83269000	6.91221400	2.58585900
H	-5.87177100	5.61942000	4.01194100
H	-7.69908700	8.00713500	0.93695500
H	-7.55823100	7.31160000	-1.44781800
H	-7.17651400	7.62012600	3.33305600
H	-9.00433800	-5.35490000	1.93652100
H	4.82912300	3.12146700	0.19767900

$S_{CT-Phen}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-6.63874400	-0.68131300	0.83753600
C	-5.24173300	-0.51853000	0.87173800
C	-4.64890500	0.68642800	0.55494700
C	-5.42145300	1.83111200	0.17843400
C	-6.82776100	1.67536500	0.14829400
C	-7.41038400	0.47249200	0.45980200
C	-3.38631400	3.08004300	-0.07149400
C	-2.64791300	1.91359200	0.30660700
C	-1.26994400	1.91631800	0.37619200
H	-0.79194000	0.98263400	0.64174400
C	-0.52132700	3.06926000	0.07638800
C	-1.26875500	4.23980100	-0.29902300
C	-2.63944100	4.24543400	-0.36627500
H	-4.58089000	-1.33951600	1.11689000
H	-7.44745200	2.52134900	-0.11655500
H	-3.16128100	5.15232900	-0.64033400
H	-8.48998700	0.41321900	0.44699400
H	-0.74710100	5.16341200	-0.50876700
N	-4.76605600	3.01262200	-0.11164500
O	-3.28691700	0.74453600	0.59869400
C	0.93748200	3.07676800	0.13851500
C	1.70145500	4.08265200	-0.50745200
C	1.66163800	2.08253200	0.84522600
C	3.08903100	4.08616100	-0.45298100
H	1.20474600	4.85263900	-1.08433600
C	3.04748100	2.09292700	0.89604300
H	1.13024100	1.30814000	1.38490500
C	3.78011200	3.09427500	0.24791500
H	3.63803500	4.86709100	-0.96850000
H	3.56422200	1.31965200	1.45452200
C	-7.27268500	-1.95539400	1.16449800
C	-8.60553500	-2.24182800	0.77221600
C	-6.59052400	-2.96627200	1.88892800
C	-9.20636300	-3.45555700	1.07908400
H	-9.16649300	-1.51840300	0.19389300
C	-7.19735500	-4.17573500	2.19277000
H	-5.58209200	-2.78989100	2.24296700

C	-8.51291700	-4.43706800	1.79216800
H	-10.22428500	-3.64101600	0.75283300
H	-6.64529300	-4.92012200	2.75667000
C	-5.53104300	4.18867400	-0.46500100
C	-5.95441200	5.08240500	0.55892900
C	-5.82567400	4.40597600	-1.78941900
C	-5.66878300	4.89026400	1.93646400
C	-6.70887400	6.23384700	0.16016000
C	-6.57066600	5.54521000	-2.16782400
H	-5.48382900	3.70073000	-2.53694300
C	-6.10888800	5.79494400	2.87284500
H	-5.09974300	4.02345600	2.24828600
C	-7.14539500	7.14503700	1.15737500
C	-7.00050400	6.43563000	-1.21524000
H	-6.79759100	5.70701300	-3.21445400
C	-6.85356300	6.93284300	2.48307700
H	-5.88397400	5.63642100	3.92113700
H	-7.71576900	8.01516900	0.85139100
H	-7.57249800	7.31098000	-1.50228000
H	-7.19221800	7.63556400	3.23523800
H	-8.98545800	-5.38207900	2.03301700
H	4.86289700	3.10127900	0.29119300

$T_{CT-Phen}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-6.64151100	-0.71606800	0.82817900
C	-5.22217800	-0.53801800	0.85321200
C	-4.64151000	0.66151300	0.56171200
C	-5.42036200	1.83046900	0.20776700
C	-6.83242600	1.67429900	0.17958000
C	-7.41938400	0.47829200	0.47068300
C	-3.37807200	3.07941200	-0.02825100
C	-2.64932800	1.91909900	0.33334800
C	-1.26428100	1.92697800	0.39833800
H	-0.77087700	0.99787700	0.65430200
C	-0.53461600	3.08494400	0.11059700
C	-1.26487000	4.24627400	-0.24945600
C	-2.64214300	4.24642500	-0.31663600
H	-4.55470000	-1.34991200	1.10676400
H	-7.44917700	2.52464900	-0.08057200
H	-3.16829300	5.15208000	-0.58560000
H	-8.49732500	0.42335200	0.43156400
H	-0.73756200	5.16924200	-0.45374400
N	-4.76093100	3.01326900	-0.08163800
O	-3.27855300	0.73895500	0.61502500
C	0.94218100	3.09584300	0.17816200
C	1.69985000	3.92642100	-0.66747800
C	1.63608900	2.27743500	1.08798300
C	3.09011000	3.93574000	-0.60677700
H	1.19889100	4.55183100	-1.39689300
C	3.02605900	2.28698300	1.14663300
H	1.08271700	1.64628600	1.77346400
C	3.76214300	3.11628200	0.29993600
H	3.65019300	4.57927800	-1.27600400
H	3.53549600	1.65194500	1.86278900

C	-7.26483300	-1.96959700	1.13116300
C	-8.68756200	-2.13493800	1.11164100
C	-6.50892000	-3.13768400	1.47324300
C	-9.28522400	-3.34890300	1.40576500
H	-9.32770100	-1.29918500	0.86354000
C	-7.11919400	-4.34261600	1.76430300
H	-5.42812200	-3.09147600	1.50815500
C	-8.51738700	-4.47272200	1.73657500
H	-10.36748700	-3.42481200	1.37811800
H	-6.50355700	-5.19965000	2.01762500
C	-5.52239900	4.18260100	-0.46215400
C	-5.95169100	5.09429400	0.54437900
C	-5.81362600	4.38149700	-1.78964200
C	-5.67406200	4.91941000	1.92562500
C	-6.70062300	6.24169900	0.12550900
C	-6.55387200	5.51604200	-2.18964500
H	-5.47075500	3.66426200	-2.52545300
C	-6.11600400	5.83810700	2.84751500
H	-5.11111100	4.05352200	2.25052600
C	-7.13917000	7.16877000	1.10816000
C	-6.98539200	6.42326100	-1.25306000
H	-6.77564100	5.66197600	-3.23971900
C	-6.85431800	6.97321200	2.43740000
H	-5.89820600	5.69333400	3.89927400
H	-7.70516100	8.03656800	0.78782500
H	-7.55335900	7.29569900	-1.55660700
H	-7.19431900	7.68739600	3.17819200
H	-8.99025900	-5.42019700	1.96565600
H	4.84494600	3.12445500	0.34710100

$T_{LE-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-6.66837500	-0.81951600	0.78021900
C	-5.27517000	-0.64908900	0.76039400
C	-4.71212600	0.60001400	0.56764600
C	-5.50874100	1.74222800	0.37184000
C	-6.89896500	1.57864400	0.43527400
C	-7.46467500	0.32353300	0.62293300
C	-3.49372300	3.06613800	0.18439500
C	-2.74440500	1.90125600	0.41424800
C	-1.35875800	1.92078800	0.42796800
H	-0.84554700	0.98067600	0.58697500
C	-0.65065400	3.10895000	0.20330600
C	-1.39754300	4.26739300	-0.05434100
C	-2.78682900	4.24578700	-0.06987500
H	-4.60357600	-1.49009500	0.87918400
H	-7.53714200	2.44745400	0.35293400
H	-3.33121900	5.15602700	-0.27503700
H	-8.54274500	0.24390900	0.68447500
H	-0.89247700	5.20924000	-0.22866000
N	-4.90537500	2.99493500	0.16675400
O	-3.33904600	0.67165700	0.59437500
C	0.83233600	3.13076900	0.22873100
C	1.55712900	3.96498500	-0.63795600

C	1.55184500	2.31856000	1.12021600
C	2.94894400	3.98717700	-0.61242000
H	1.02886400	4.58449700	-1.35335000
C	2.94378600	2.33998500	1.14427700
H	1.01808800	1.68156600	1.81610300
C	3.64944400	3.17471300	0.27850900
H	3.48696500	4.63412800	-1.29619300
H	3.47723800	1.70932000	1.84659000
C	-7.27086300	-2.15896700	0.98433800
C	-8.46856400	-2.51391400	0.34207400
C	-6.66380600	-3.10799300	1.82304700
C	-9.03804200	-3.76984400	0.53263200
H	-8.94580500	-1.80978500	-0.32955500
C	-7.23333200	-4.36413100	2.01251600
H	-5.75142400	-2.85392500	2.34997500
C	-8.42333100	-4.70146100	1.36857600
H	-9.95906300	-4.02377500	0.02003700
H	-6.75047200	-5.07746300	2.67092700
C	-5.70455500	4.10429300	-0.20733400
C	-5.79712900	5.26672500	0.62670100
C	-6.42118800	4.02746000	-1.47350600
C	-5.25094800	5.33743400	1.91846000
C	-6.52935000	6.40373100	0.12055400
C	-7.09708900	5.11664100	-1.93588900
H	-6.34473900	3.11939900	-2.05816300
C	-5.36479000	6.52031300	2.70817200
H	-4.73619400	4.47716700	2.32755500
C	-6.63025300	7.55322000	0.92290100
C	-7.15252600	6.31902100	-1.15823500
H	-7.59022400	5.08511400	-2.90055400
C	-6.03752700	7.61198600	2.21715700
H	-4.91227000	6.54430100	3.69268200
H	-7.18224200	8.40741200	0.54624600
H	-7.69989700	7.17660500	-1.53175500
H	-6.12783800	8.51814100	2.80497600
H	-8.86654000	-5.67953000	1.51633500
H	4.73307200	3.19169800	0.29761500

$T_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-6.58532000	-0.54048100	0.95346400
C	-5.18863300	-0.43332500	0.91594900
C	-4.57188500	0.77866600	0.64896700
C	-5.31566900	1.94631500	0.41513300
C	-6.70959900	1.83295700	0.42262900
C	-7.32950200	0.61881600	0.69176900
C	-3.23798600	3.13979400	0.08795200
C	-2.54091700	1.93672500	0.29866800
C	-1.15931600	1.88372300	0.24694700
H	-0.68761400	0.92003100	0.39229800
C	-0.39982500	3.03689900	-0.00558400
C	-1.09073700	4.24449100	-0.17799400
C	-2.47797900	4.29841100	-0.12059000
H	-4.55319200	-1.29771700	1.06262700

H	-7.31341100	2.70598700	0.22223900
H	-2.98191000	5.24959700	-0.22153000
H	-8.41154600	0.58395600	0.71459300
H	-0.54107200	5.16613100	-0.32226300
N	-4.64260600	3.15731100	0.13461300
O	-3.19589600	0.76147300	0.58315800
C	1.08069900	2.97780100	-0.06321700
C	1.79934300	3.79920500	-0.94743200
C	1.80476200	2.10146400	0.76167600
C	3.18938100	3.74693100	-1.00333100
H	1.26520800	4.46737300	-1.61294400
C	3.19476700	2.04899500	0.70459600
H	1.27859200	1.47216600	1.47008200
C	3.89422500	2.87150700	-0.17786400
H	3.72188200	4.38521200	-1.69943000
H	3.73240000	1.36988600	1.35671800
C	-7.24416500	-1.83632200	1.24866900
C	-8.45007600	-2.19208000	0.62294500
C	-6.68029200	-2.74245800	2.16139400
C	-9.06924700	-3.40764500	0.90092800
H	-8.89540900	-1.52287300	-0.10397200
C	-7.29918300	-3.95859300	2.43804100
H	-5.76186800	-2.48428200	2.67589800
C	-8.49694000	-4.29727000	1.80954700
H	-9.99597700	-3.66362900	0.39973400
H	-6.84862800	-4.63886900	3.15202500
C	-5.34180400	4.32731000	-0.25452400
C	-6.17970900	5.03292800	0.67036400
C	-5.19005800	4.78188000	-1.63047700
C	-6.24740600	4.72906700	2.03976200
C	-6.95852800	6.13954500	0.16657000
C	-5.94320100	5.82207000	-2.08646100
H	-4.52522800	4.23477300	-2.28691500
C	-7.10245000	5.45715900	2.91959500
H	-5.63653200	3.92924700	2.43915400
C	-7.78761000	6.84241600	1.05750400
C	-6.84292500	6.50618100	-1.20582900
H	-5.87454600	6.13384300	-3.12225000
C	-7.86441500	6.49235500	2.43640500
H	-7.14330400	5.18006800	3.96657700
H	-8.37157400	7.67573800	0.68231100
H	-7.43126200	7.33716800	-1.57715600
H	-8.52129900	7.05092800	3.09313000
H	-8.97885800	-5.24394500	2.02514000
H	4.97646700	2.83049000	-0.22200700

S16 Coordinates of the optimized geometries of molecule 2

S_0 geometry (Å) (B3LYP/6-311G(d,p))

C	-1.66491800	-4.30680000	1.05994700
C	-2.36690200	-3.15506500	0.71038400
C	-1.69732500	-1.98653100	0.33879600
C	-0.29222900	-2.01922800	0.32969700

C	0.40482700	-3.16215600	0.67347100
C	-0.26661300	-4.33906200	1.05019700
C	-0.20343200	0.24078400	-0.39250900
C	-1.60676600	0.31958000	-0.39774200
C	-2.18301800	1.53178200	-0.78556300
H	-3.26068500	1.62177200	-0.81115800
C	-1.39313000	2.61987500	-1.15093600
C	0.58078100	1.31869000	-0.75790200
H	-2.22646600	-5.19592600	1.31894000
H	-3.44854800	-3.16663000	0.71666000
H	1.48663300	-3.11124300	0.66516300
H	-1.88378300	3.53239800	-1.46646600
H	1.65581900	1.19563600	-0.71100100
N	-2.36236000	-0.80010900	-0.01241700
O	0.45981400	-0.90963300	-0.00823700
C	0.48614200	-5.56195800	1.41633300
C	0.00923800	-6.44376700	2.39955800
C	1.70305000	-5.88513000	0.79498000
C	0.71303400	-7.59172300	2.74234600
H	-0.91805400	-6.22279700	2.91528700
C	2.40741600	-7.03249400	1.13916200
H	2.10002500	-5.23876800	0.02079100
C	1.92958300	-7.91373800	2.12112300
H	0.30374500	-8.25367400	3.49684400
H	3.35022200	-7.23834000	0.64550600
C	2.68269700	-9.13907100	2.48981700
C	2.72421000	-9.58887000	3.81946500
C	3.37432100	-9.88186400	1.51928600
C	3.43043100	-10.73802400	4.16544900
H	2.21788000	-9.02262100	4.59271700
C	4.08092300	-11.03075800	1.86539800
H	3.34108400	-9.57014500	0.48166800
C	4.11242200	-11.46475300	3.19017600
H	3.45418700	-11.06135800	5.20013800
H	4.60097800	-11.59195500	1.09709300
C	0.00332800	2.54081800	-1.14624100
H	4.66234800	-12.35920000	3.45954400
C	-3.79763200	-0.75134900	-0.03650000
C	-4.50987800	-0.34888600	1.13302000
C	-4.46781900	-1.09358100	-1.18812900
C	-5.94093800	-0.31067100	1.07466300
C	-3.86284000	0.01271800	2.34385300
C	-5.87929800	-1.05372500	-1.23729700
H	-3.90101100	-1.39538000	-2.06099800
C	-6.59780800	-0.67099800	-0.13111100
C	-6.66431900	0.08829800	2.23006800
C	-4.59576400	0.39363100	3.44273400
H	-2.78160900	-0.01495800	2.39254300
H	-6.38778600	-1.32734400	-2.15404900
H	-7.68139900	-0.63906800	-0.16432100
C	-6.00893700	0.43250100	3.38733200
H	-7.74747700	0.11632700	2.18162700
H	-4.08906900	0.66719900	4.36108400
H	-6.57173200	0.73528100	4.26272700

C	0.84859900	3.69300100	-1.53822800
C	0.45593800	5.01221800	-1.25983100
C	2.07193200	3.51034500	-2.20284000
C	1.24505000	6.09393500	-1.63092000
H	-0.46480500	5.19524900	-0.71822000
C	2.86236100	4.59230900	-2.57104900
H	2.39784200	2.51011200	-2.46377600
C	2.46781300	5.91049900	-2.29509500
H	0.92011800	7.09496500	-1.37148500
H	3.78559800	4.40977200	-3.10886500
C	3.31173300	7.06649800	-2.68960000
C	2.73210400	8.26628300	-3.13296700
C	4.71279900	6.99199100	-2.63058200
C	3.52353700	9.35061900	-3.50292400
H	1.65367100	8.34408100	-3.20983800
C	5.50425200	8.07600000	-3.00146000
H	5.18653800	6.08585200	-2.27079000
C	4.91361800	9.26083900	-3.43932700
H	3.05314800	10.26414200	-3.84918700
H	6.58394200	7.99717200	-2.94032200
H	5.52971600	10.10480800	-3.72770400

$S_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.65381000	-4.27481300	1.04660900
C	-2.35088800	-3.14037200	0.69305900
C	-1.66352800	-1.97947700	0.29288100
C	-0.25022100	-2.02646700	0.26655900
C	0.44729700	-3.16935600	0.62052800
C	-0.23869500	-4.31998800	1.01873900
C	-0.16213700	0.21173100	-0.45148800
C	-1.57417600	0.28995000	-0.43459900
C	-2.16765000	1.51327600	-0.79711000
H	-3.24540800	1.58401900	-0.80075000
C	-1.38342200	2.58943800	-1.15053900
C	0.62310700	1.29482800	-0.80986200
H	-2.21017100	-5.15879300	1.32862100
H	-3.43076400	-3.12314100	0.70611300
H	1.52812900	-3.12954900	0.60080200
H	-1.86852000	3.51050600	-1.44529800
H	1.69765500	1.17400100	-0.77809900
N	-2.31987700	-0.81642300	-0.06824200
O	0.48171100	-0.93737700	-0.10150700
C	0.49100100	-5.54852400	1.39493700
C	-0.01192600	-6.41794400	2.37640600
C	1.71106500	-5.88463300	0.78614900
C	0.67860000	-7.56705800	2.73689800
H	-0.94284200	-6.18669700	2.87988600
C	2.39584700	-7.03803500	1.14261300
H	2.12240600	-5.24900600	0.01119000
C	1.89739900	-7.90501100	2.12809400
H	0.25580200	-8.21921500	3.49174300
H	3.33940100	-7.25995600	0.65851500
C	2.63279400	-9.13535500	2.51227200

C	2.65391700	-9.57555100	3.84544300
C	3.32652000	-9.89025800	1.55291200
C	3.34529900	-10.72881800	4.20626700
H	2.14536100	-8.99897800	4.60938500
C	4.01583500	-11.04469700	1.91402800
H	3.30765400	-9.58504400	0.51312400
C	4.02885800	-11.46895200	3.24225300
H	3.35561500	-11.04538600	5.24310900
H	4.53737400	-11.61714400	1.15530200
C	0.03019600	2.50884700	-1.16719600
H	4.56636900	-12.36728200	3.52327900
C	-3.76847900	-0.75776100	-0.06317700
C	-4.43249700	-0.35904800	1.13303400
C	-4.45167100	-1.10130200	-1.25482300
C	-5.88155900	-0.31578100	1.08927500
C	-3.77521900	-0.01105700	2.33579000
C	-5.83569800	-1.05025500	-1.26754700
H	-3.88821300	-1.39703100	-2.13163900
C	-6.54827100	-0.66521500	-0.12027600
C	-6.57152400	0.07502000	2.26114800
C	-4.50255400	0.37220700	3.47858700
H	-2.69293300	-0.03856500	2.38360100
H	-6.37250000	-1.31086300	-2.17367000
H	-7.63221800	-0.62869200	-0.14203400
C	-5.88993700	0.41433600	3.44003300
H	-7.65630700	0.10866400	2.23356800
H	-3.97103200	0.63370300	4.38736700
H	-6.45190000	0.70960000	4.32017500
C	0.85393800	3.67271500	-1.55459800
C	0.43472300	4.98291600	-1.27206600
C	2.08242000	3.50690600	-2.21458200
C	1.21239200	6.07625900	-1.62844900
H	-0.49124000	5.15144900	-0.73564700
C	2.85486400	4.60175700	-2.57643500
H	2.42328000	2.51361100	-2.48103100
C	2.43940100	5.91215900	-2.29036300
H	0.87359300	7.07058600	-1.36325600
H	3.78047600	4.43696900	-3.11485400
C	3.26774400	7.08192000	-2.67468300
C	2.67117800	8.27697700	-3.10756900
C	4.66934500	7.02346100	-2.61485500
C	3.44875500	9.37400000	-3.46843500
H	1.59199300	8.34137500	-3.18463000
C	5.44635000	8.12142200	-2.97408000
H	5.15465400	6.12052500	-2.26283600
C	4.83973100	9.30145000	-3.40292700
H	2.96717800	10.28400000	-3.80806200
H	6.52678500	8.05698800	-2.91184400
H	5.44487600	10.15592900	-3.68323600

$S_{CT-Biph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.65372800	-4.27475700	1.04692800
C	-2.35084100	-3.14034800	0.69336100

C	-1.66352900	-1.97949100	0.29295000
C	-0.25021000	-2.02650900	0.26642800
C	0.44733300	-3.16938300	0.62037900
C	-0.23862500	-4.31996200	1.01881900
C	-0.16218600	0.21167900	-0.45166700
C	-1.57423800	0.28992600	-0.43458000
C	-2.16771800	1.51331200	-0.79692700
H	-3.24547500	1.58407200	-0.80041400
C	-1.38350800	2.58947500	-1.15038000
C	0.62302700	1.29477400	-0.81009000
H	-2.21003500	-5.15870800	1.32914700
H	-3.43071500	-3.12307700	0.70657200
H	1.52816400	-3.12965600	0.60049000
H	-1.86859600	3.51059800	-1.44499200
H	1.69758200	1.17396100	-0.77850600
N	-2.31989400	-0.81646700	-0.06822500
O	0.48162200	-0.93747200	-0.10187300
C	0.49111200	-5.54848200	1.39500100
C	-0.01158600	-6.41769700	2.37677100
C	1.71097600	-5.88475400	0.78591300
C	0.67898700	-7.56677600	2.73727700
H	-0.94234800	-6.18628400	2.88045900
C	2.39580300	-7.03812500	1.14239000
H	2.12210100	-5.24927400	0.01072100
C	1.89759600	-7.90488800	2.12817900
H	0.25640200	-8.21877700	3.49237700
H	3.33920500	-7.26020500	0.65806600
C	2.63305900	-9.13519000	2.51238200
C	2.65460500	-9.57508900	3.84564300
C	3.32643000	-9.89033700	1.55295800
C	3.34605700	-10.72830600	4.20649600
H	2.14633000	-8.99831400	4.60962100
C	4.01581600	-11.04472400	1.91410400
H	3.30722500	-9.58535100	0.51311100
C	4.02926400	-11.46868100	3.24241900
H	3.35670900	-11.04464300	5.24340400
H	4.53707900	-11.61736700	1.15533500
C	0.03009900	2.50884100	-1.16724700
H	4.56683000	-12.36697300	3.52346600
C	-3.76847700	-0.75785300	-0.06318100
C	-4.43262400	-0.35920600	1.13300700
C	-4.45166600	-1.10128700	-1.25489400
C	-5.88165700	-0.31597700	1.08916000
C	-3.77539000	-0.01126800	2.33578600
C	-5.83567800	-1.05026300	-1.26767700
H	-3.88819500	-1.39694500	-2.13172500
C	-6.54836300	-0.66533200	-0.12041500
C	-6.57171400	0.07473700	2.26102800
C	-4.50279600	0.37190500	3.47857300
H	-2.69310900	-0.03873400	2.38362900
H	-6.37240400	-1.31080900	-2.17387100
H	-7.63229900	-0.62881800	-0.14218400
C	-5.89018600	0.41398800	3.43994400
H	-7.65649200	0.10835300	2.23336400

H	-3.97135600	0.63336300	4.38741100
H	-6.45217800	0.70917900	4.32009500
C	0.85381800	3.67270900	-1.55468800
C	0.43473700	4.98289400	-1.27186700
C	2.08213900	3.50690600	-2.21496700
C	1.21239900	6.07623700	-1.62825500
H	-0.49110200	5.15137700	-0.73521500
C	2.85457600	4.60176200	-2.57682400
H	2.42284900	2.51362000	-2.48164300
C	2.43925500	5.91214100	-2.29045400
H	0.87375200	7.07055900	-1.36284700
H	3.78005900	4.43702900	-3.11548200
C	3.26760500	7.08190500	-2.67477100
C	2.67102800	8.27702300	-3.10746700
C	4.66920900	7.02337100	-2.61512400
C	3.44860700	9.37404500	-3.46833300
H	1.59183400	8.34146000	-3.18437200
C	5.44621500	8.12133200	-2.97434900
H	5.15450900	6.12037200	-2.26325500
C	4.83958800	9.30142400	-3.40300900
H	2.96703500	10.28410100	-3.80781900
H	6.52665500	8.05685600	-2.91225500
H	5.44473500	10.15590200	-3.68331700

$T_{CT-Biph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.67802900	-4.29244400	1.06770500
C	-2.37858000	-3.15066800	0.73224100
C	-1.70174500	-1.98415500	0.33147900
C	-0.29009500	-2.02948000	0.28290400
C	0.40745500	-3.17901300	0.61847100
C	-0.26536000	-4.33908600	1.01952000
C	-0.18055500	0.22647000	-0.42820300
C	-1.61805300	0.30742200	-0.39819400
C	-2.19810900	1.54851200	-0.76426800
H	-3.27548600	1.64766500	-0.75512500
C	-1.42399300	2.61316100	-1.12847200
C	0.60110700	1.28360800	-0.79202500
H	-2.23564500	-5.17687500	1.34768800
H	-3.45932800	-3.15217500	0.76555200
H	1.48855300	-3.13667300	0.58232600
H	-1.92531700	3.53065200	-1.39953600
H	1.67006900	1.12381700	-0.78079000
N	-2.34954700	-0.80507300	-0.01325300
O	0.44953900	-0.93835600	-0.08438700
C	0.47574300	-5.56662200	1.37690200
C	-0.01852900	-6.46220400	2.34082300
C	1.70212900	-5.88510200	0.76862000
C	0.67971200	-7.61341900	2.68074000
H	-0.95293100	-6.24934200	2.84645100
C	2.39807400	-7.03753000	1.10806100
H	2.11164700	-5.23269900	0.00643700
C	1.90506000	-7.93016700	2.07330200
H	0.25808700	-8.28367800	3.42076900

H	3.34664600	-7.23941500	0.62420700
C	2.65027900	-9.16076200	2.43713500
C	2.66293300	-9.63323100	3.75974100
C	3.36394300	-9.88653500	1.46936700
C	3.36281900	-10.78734000	4.10144500
H	2.13961300	-9.08068300	4.53152800
C	4.06362400	-11.04070100	1.81135400
H	3.35308200	-9.55782100	0.43658900
C	4.06671000	-11.49695800	3.12905400
H	3.36449800	-11.12805600	5.13078400
H	4.60075000	-11.58854400	1.04519800
C	0.03587700	2.54716100	-1.16572800
H	4.61159700	-12.39542100	3.39519700
C	-3.79391900	-0.74240000	0.01257000
C	-4.45494800	-0.34544800	1.21033200
C	-4.49233100	-1.06759300	-1.12476900
C	-5.88684800	-0.29846800	1.19429200
C	-3.76781900	0.00091300	2.40336000
C	-5.90391700	-1.01697200	-1.12766700
H	-3.95352200	-1.36343500	-2.01674600
C	-6.58268300	-0.64173400	0.00574300
C	-6.57222200	0.09321100	2.37486100
C	-4.46602400	0.37519300	3.52661300
H	-2.68572300	-0.03030700	2.42408500
H	-6.44258800	-1.27692800	-2.03063900
H	-7.66634100	-0.60240900	0.00756900
C	-5.87988900	0.42219000	3.51454300
H	-7.65597000	0.12799200	2.35900400
H	-3.93001200	0.63759700	4.43126900
H	-6.41371800	0.71968100	4.40949200
C	0.83645900	3.65932000	-1.54627600
C	0.27076400	4.93354400	-1.89560100
C	2.27078600	3.59627200	-1.61035600
C	1.04890100	6.00517300	-2.26481000
H	-0.80069800	5.07847000	-1.85867900
C	3.03743600	4.67573700	-1.97325100
H	2.78066600	2.66932400	-1.38134000
C	2.46627200	5.93260900	-2.32032000
H	0.55388500	6.94330300	-2.48806900
H	4.11229700	4.54599100	-2.02516500
C	3.29024100	7.08003000	-2.71013800
C	2.76794300	8.13396300	-3.49486600
C	4.64490000	7.18525000	-2.31894500
C	3.55041900	9.22217600	-3.86188700
H	1.74371400	8.08617000	-3.84458600
C	5.42483600	8.27432200	-2.68935900
H	5.08428500	6.41753600	-1.69356400
C	4.88663200	9.30423000	-3.46383500
H	3.11744900	10.00794300	-4.47172200
H	6.45821600	8.32479200	-2.36320300
H	5.49592800	10.15315900	-3.75155000

$T_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.60567800	-4.35065900	1.29097600

C	-2.31722700	-3.19407800	0.99712700
C	-1.66783400	-2.04774300	0.51995200
C	-0.26675900	-2.09697700	0.40623400
C	0.44259500	-3.24623600	0.70499000
C	-0.21250900	-4.40817500	1.14426500
C	-0.20472100	0.17118000	-0.25716300
C	-1.60420300	0.26253300	-0.19042900
C	-2.18857400	1.47411800	-0.57391800
H	-3.26511800	1.56404900	-0.58035700
C	-1.40823500	2.55668600	-0.95933100
C	0.57533900	1.25001200	-0.64185200
H	-2.15152200	-5.22236100	1.62910700
H	-3.38912600	-3.17499100	1.13628000
H	1.52093800	-3.20777600	0.61621400
H	-1.90415900	3.46897100	-1.26633000
H	1.64946700	1.11378500	-0.64842900
N	-2.35850200	-0.86494700	0.20463000
O	0.46742100	-0.99576200	0.03228500
C	0.54954100	-5.64000100	1.45360500
C	0.14370800	-6.51019400	2.47809300
C	1.70486400	-5.98214200	0.73290400
C	0.85802300	-7.66621000	2.76641700
H	-0.73302000	-6.27417100	3.06965600
C	2.41816600	-7.13886900	1.02136200
H	2.04414400	-5.34458000	-0.07515500
C	2.01223200	-8.00865900	2.04510400
H	0.50502200	-8.31894400	3.55638000
H	3.31231200	-7.36116500	0.45058500
C	2.77547800	-9.24398400	2.35402300
C	2.92381200	-9.68940600	3.67742200
C	3.36991600	-10.00037800	1.33114200
C	3.63984200	-10.84797900	3.96696400
H	2.49449400	-9.11261700	4.48853700
C	4.08587200	-11.15893900	1.62087300
H	3.25220700	-9.69183300	0.29874800
C	4.22445200	-11.58844000	2.94019700
H	3.74761000	-11.16805600	4.99729100
H	4.52936400	-11.73094000	0.81355500
C	-0.00811400	2.47490500	-0.99319600
H	4.78189400	-12.49032900	3.16571600
C	-3.77500700	-0.87244600	0.15180400
C	-4.55634800	-0.06062400	1.03863300
C	-4.41028000	-1.72941300	-0.84021600
C	-5.98642800	-0.02996500	0.84093000
C	-4.00811000	0.66628600	2.10771500
C	-5.76063100	-1.67580100	-1.01580000
H	-3.78241000	-2.34720700	-1.46983200
C	-6.56494700	-0.82195300	-0.19292300
C	-6.76977600	0.76075300	1.69913900
C	-4.82798000	1.46451600	2.95961500
H	-2.94252100	0.61943900	2.29388000
H	-6.23576700	-2.27170800	-1.78645000
H	-7.63886700	-0.79307800	-0.33583000
C	-6.18500100	1.51635000	2.75564600

H	-7.84442400	0.78288300	1.55464200
H	-4.36575100	2.02791400	3.76183200
H	-6.81870600	2.12226400	3.39290000
C	0.82423700	3.62987900	-1.40290700
C	0.43935100	4.94540200	-1.09891300
C	2.02473500	3.45274700	-2.10885500
C	1.21666400	6.03074900	-1.48358900
H	-0.46382300	5.12260800	-0.52674500
C	2.80194900	4.53852000	-2.49250100
H	2.34151800	2.45533400	-2.39067300
C	2.41665200	5.85363300	-2.18952500
H	0.90079400	7.02901800	-1.20356700
H	3.70649100	4.36205200	-3.06291900
C	3.24724800	7.01359600	-2.60013800
C	2.65325400	8.21715800	-3.01283000
C	4.64935400	6.93858500	-2.58704500
C	3.43231300	9.30513900	-3.39781000
H	1.57291800	8.29518600	-3.05417600
C	5.42833600	8.02646200	-2.97246500
H	5.13434600	6.02912700	-2.25150300
C	4.82367500	9.21513300	-3.37961200
H	2.95108100	10.22175700	-3.72009300
H	6.50942200	7.94756100	-2.94681200
H	5.43012200	10.06207600	-3.67948100

$T_{LE-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.59889500	-4.35306800	1.29386500
C	-2.31268800	-3.19765600	1.00073500
C	-1.66585000	-2.05046600	0.52218800
C	-0.26487700	-2.09759300	0.40620300
C	0.44672400	-3.24565600	0.70413500
C	-0.20587900	-4.40846900	1.14493500
C	-0.20734100	0.17051500	-0.25778300
C	-1.60685300	0.25976200	-0.18881800
C	-2.19364800	1.47036500	-0.57167600
H	-3.27033800	1.55871200	-0.57654200
C	-1.41556100	2.55408100	-0.95853300
C	0.57047800	1.25043200	-0.64388800
H	-2.14291100	-5.22542900	1.63323800
H	-3.38440300	-3.18028200	1.14155300
H	1.52485000	-3.20558800	0.61338900
H	-1.91343600	3.46551500	-1.26489200
H	1.64478300	1.11570100	-0.65228700
N	-2.35875400	-0.86876500	0.20777400
O	0.46699300	-0.99538400	0.03071200
C	0.55862100	-5.63896600	1.45359500
C	0.15539400	-6.50969700	2.47869100
C	1.71378900	-5.97924100	0.73171600
C	0.87205900	-7.66440000	2.76650400
H	-0.72113900	-6.27519400	3.07113700
C	2.42944000	-7.13467100	1.01965000
H	2.05116800	-5.34131300	-0.07683600
C	2.02614900	-8.00497400	2.04404500

H	0.52100300	-8.31744300	3.55706300
H	3.32327400	-7.35546100	0.44780700
C	2.79196200	-9.23885900	2.35250000
C	2.94110200	-9.68458300	3.67574800
C	3.38814000	-9.99355900	1.32933500
C	3.65958200	-10.84177200	3.96485300
H	2.51038700	-9.10923500	4.48713600
C	4.10654000	-11.15073900	1.61863700
H	3.27003800	-9.68482300	0.29705400
C	4.24591200	-11.58053500	2.93781000
H	3.76787100	-11.16208700	4.99504400
H	4.55135900	-11.72139400	0.81110600
C	-0.01536600	2.47443100	-0.99455800
H	4.80525100	-12.48132700	3.16299100
C	-3.77535300	-0.87825600	0.15752000
C	-4.55610700	-0.06755800	1.04590800
C	-4.41133000	-1.73595400	-0.83336000
C	-5.98663200	-0.03885900	0.85098800
C	-4.00674400	0.65996300	2.11398000
C	-5.76208500	-1.68425100	-1.00631500
H	-3.78380800	-2.35270000	-1.46434800
C	-6.56609400	-0.83161100	-0.18167600
C	-6.76941300	0.75079900	1.71077700
C	-4.82606500	1.45711400	2.96756600
H	-2.94075100	0.61443100	2.29815600
H	-6.23790500	-2.28063700	-1.77616100
H	-7.64033500	-0.80440800	-0.32240800
C	-6.18354000	1.50715600	2.76620000
H	-7.84436300	0.77148300	1.56840300
H	-4.36302500	2.02110300	3.76889000
H	-6.81680500	2.11224000	3.40466800
C	0.81464300	3.63055400	-1.40583100
C	0.42741200	4.94573000	-1.10314100
C	2.01524900	3.45494600	-2.11204200
C	1.20254400	6.03213400	-1.48928500
H	-0.47590100	5.12199400	-0.53092300
C	2.79028400	4.54177700	-2.49715500
H	2.33395600	2.45788500	-2.39288200
C	2.40264400	5.85653200	-2.19547700
H	0.88474700	7.03005700	-1.21024200
H	3.69498200	4.36625200	-3.06759900
C	3.23097600	7.01761500	-2.60757800
C	2.63465900	8.22029500	-3.01961300
C	4.63324100	6.94459200	-2.59657400
C	3.41162500	9.30932500	-3.40593600
H	1.55416800	8.29694000	-3.05930000
C	5.41011500	8.03352000	-2.98335600
H	5.12011300	6.03589200	-2.26172100
C	4.80316200	9.22129000	-3.38980700
H	2.92860400	10.22520400	-3.72761700
H	6.49134000	7.95611600	-2.95933000
H	5.40795800	10.06903700	-3.69071800

S17 Coordinates of the optimized geometries of molecule 3

S_0 geometry (Å) (B3LYP/6-311G(d,p))

C	-1.52448200	-4.34477700	0.79956800
C	-2.16455700	-3.14409600	0.51334100
C	-1.50511700	-1.91611500	0.66092600
C	-0.17461800	-1.94874600	1.11618200
C	0.47269600	-3.15479600	1.36020000
C	-0.18896300	-4.38286100	1.21809600
C	-0.07244600	0.63039700	0.29035800
C	-1.41185500	0.43517500	-0.09214400
C	-1.98472500	1.39319000	-0.93988900
H	-3.01285300	1.28462200	-1.25421400
C	-1.25398400	2.48792500	-1.38796100
C	0.66507100	1.70431200	-0.19533200
H	-2.07270800	-5.26851100	0.65795000
H	-3.18933900	-3.16463100	0.17128300
H	1.49743200	-3.13066600	1.71213400
H	-1.73758800	3.19483900	-2.05152600
H	1.69323500	1.81513800	0.12885300
N	-2.14386100	-0.68412100	0.37552400
C	0.50288700	-5.66472000	1.50191400
C	-0.18191800	-6.73974900	2.09130300
C	1.86047900	-5.83890400	1.18802700
C	0.46603300	-7.94381300	2.35468100
H	-1.22427200	-6.62550000	2.36589600
C	2.50907000	-7.04194900	1.45448500
H	2.40802600	-5.03415100	0.71086300
C	1.81501300	-8.10093600	2.03852400
H	-0.08227900	-8.75741700	2.81632200
H	3.55629100	-7.15457400	1.19693400
C	0.08994600	2.66610900	-1.03813600
C	-3.58039200	-0.66253900	0.26421800
C	-4.34746600	-0.26569700	1.40128500
C	-4.20156600	-1.01612500	-0.91225500
C	-5.77557600	-0.24543500	1.28397600
C	-3.75709700	0.10799500	2.63757200
C	-5.61023900	-0.99411100	-1.01968700
H	-3.60028900	-1.31403200	-1.76324900
C	-6.37870900	-0.61721900	0.05416500
C	-6.55159000	0.14794200	2.40686000
C	-4.53996300	0.48306000	3.70334000
H	-2.67851300	0.09318000	2.72894300
H	-6.07635000	-1.27693600	-1.95598800
H	-7.46032600	-0.59884200	-0.02374300
C	-5.94999700	0.50408500	3.58925900
H	-7.63207300	0.16197900	2.31287100
H	-4.07525200	0.76583400	4.64098700
H	-6.55279000	0.80248700	4.43922100
C	0.87739700	3.82246000	-1.53326400
C	0.28357500	5.08514600	-1.69129800
C	2.23669100	3.68655400	-1.85845900
C	1.02062100	6.17003900	-2.15888500
H	-0.75792900	5.22460100	-1.42536600

C	2.97443100	4.77239500	-2.32287100
H	2.71538200	2.71811200	-1.76868700
C	2.37007300	6.01957800	-2.47626000
H	0.54152700	7.13679600	-2.26641300
H	4.02110000	4.64102000	-2.57371300
S	0.65619500	-0.42541000	1.52972200
H	2.31956600	-9.03783400	2.24495700
H	2.94408900	6.86457200	-2.83882500

$S_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.60446300	-4.28781900	1.17486200
C	-2.16275900	-3.09725500	0.77215300
C	-1.35875000	-1.98524000	0.43123700
C	0.04729200	-2.15453800	0.52121200
C	0.59797000	-3.37231200	0.93037500
C	-0.20403800	-4.45961100	1.26347700
C	0.15004600	0.44184600	-0.30752400
C	-1.26620200	0.35386500	-0.31374300
C	-1.97993700	1.51303900	-0.69599000
H	-3.05744900	1.46735100	-0.71911800
C	-1.32806600	2.67238200	-1.04567000
C	0.79636000	1.62757700	-0.66766300
H	-2.26114200	-5.11673800	1.40546800
H	-3.23433800	-2.99662600	0.69965600
H	1.67538500	-3.45219900	1.00802500
H	-1.91823700	3.52655700	-1.35148500
H	1.87829200	1.65807300	-0.62708400
N	-1.96361300	-0.79871900	0.03083000
C	0.38596900	-5.74750500	1.69309200
C	-0.25134300	-6.53825400	2.66295700
C	1.59386800	-6.20740500	1.14384700
C	0.30489600	-7.74582300	3.07374100
H	-1.17328600	-6.19592300	3.11787900
C	2.14573700	-7.41756500	1.55234800
H	2.09100200	-5.62929500	0.37373800
C	1.50460300	-8.19079100	2.51977500
H	-0.19676000	-8.33671900	3.83132700
H	3.07351200	-7.76048300	1.10914700
C	0.08292000	2.76152900	-1.04419800
C	-3.41822100	-0.75970500	-0.02823000
C	-4.13918500	-0.36370700	1.13376800
C	-4.04467500	-1.11940800	-1.24489600
C	-5.58552700	-0.33987900	1.02841600
C	-3.53874000	0.00051100	2.36192900
C	-5.42781500	-1.08751100	-1.31856800
H	-3.44020600	-1.41227600	-2.09507300
C	-6.19496400	-0.70561900	-0.20643600
C	-6.33041400	0.04883700	2.16671100
C	-4.31967200	0.38070100	3.46987100
H	-2.45927700	-0.01229100	2.45544200
H	-5.92093100	-1.36079300	-2.24562800
H	-7.27735700	-0.68396300	-0.27530100
C	-5.70443100	0.40417800	3.37182500
H	-7.41335100	0.06777400	2.09229700

H	-3.83130100	0.65463700	4.39905200
H	-6.30741200	0.69712500	4.22522400
C	0.77381200	4.01243500	-1.43066100
C	0.21494600	5.26356700	-1.12307500
C	2.00135000	3.97834000	-2.11210000
C	0.86565900	6.44058100	-1.48024300
H	-0.72070900	5.31814000	-0.57940400
C	2.64795700	5.15634800	-2.47258300
H	2.44038000	3.02615800	-2.38574800
C	2.08373100	6.39202700	-2.15707500
H	0.42302900	7.39635700	-1.22466500
H	3.58957800	5.10896900	-3.00725100
S	1.18742100	-0.88492900	0.15192500
H	1.93564200	-9.13286300	2.83811700
H	2.58836000	7.30918900	-2.43773200

$S_{CT-Phen}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.60451100	-4.28756000	1.17522800
C	-2.16274500	-3.09693900	0.77259200
C	-1.35868700	-1.98498700	0.43169300
C	0.04730900	-2.15429000	0.52167400
C	0.59795200	-3.37217900	0.93063800
C	-0.20408700	-4.45945500	1.26371300
C	0.15012600	0.44207300	-0.30703100
C	-1.26611900	0.35408200	-0.31343600
C	-1.97976400	1.51321400	-0.69600300
H	-3.05727200	1.46753400	-0.71935700
C	-1.32784200	2.67251700	-1.04571300
C	0.79650100	1.62775000	-0.66732300
H	-2.26126100	-5.11641900	1.40585300
H	-3.23432900	-2.99621300	0.70014400
H	1.67537600	-3.45215500	1.00812900
H	-1.91799200	3.52664000	-1.35172900
H	1.87844400	1.65817800	-0.62677300
N	-1.96353300	-0.79848300	0.03119500
C	0.38589000	-5.74743600	1.69311700
C	-0.25135000	-6.53822300	2.66300300
C	1.59369800	-6.20734500	1.14370900
C	0.30486100	-7.74586100	3.07361600
H	-1.17321600	-6.19586100	3.11806200
C	2.14555600	-7.41756800	1.55205700
H	2.09079200	-5.62919100	0.37360300
C	1.50448600	-8.19084700	2.51947600
H	-0.19674300	-8.33680300	3.83120100
H	3.07327700	-7.76047800	1.10873300
C	0.08314600	2.76168200	-1.04403800
C	-3.41816000	-0.75973300	-0.02816800
C	-4.13941800	-0.36385600	1.13365700
C	-4.04423400	-1.11959800	-1.24493700
C	-5.58578700	-0.34026900	1.02792800
C	-3.53934200	0.00049600	2.36191900
C	-5.42735800	-1.08793500	-1.31899700
H	-3.43941700	-1.41242400	-2.09488500

C	-6.19481600	-0.70611100	-0.20703200
C	-6.33099000	0.04834700	2.16605900
C	-4.32060200	0.38058800	3.46968600
H	-2.45989700	-0.01209500	2.45570800
H	-5.92026500	-1.36131600	-2.24613100
H	-7.27719600	-0.68462000	-0.27621100
C	-5.70533900	0.40381300	3.37129600
H	-7.41391400	0.06711600	2.09142900
H	-3.83244200	0.65462700	4.39894300
H	-6.30861500	0.69666900	4.22452100
C	0.77409100	4.01252900	-1.43054400
C	0.21524100	5.26368800	-1.12302600
C	2.00167900	3.97838200	-2.11187300
C	0.86600700	6.44067700	-1.48018300
H	-0.72044600	5.31828800	-0.57940900
C	2.64834500	5.15636600	-2.47234200
H	2.44072900	3.02617300	-2.38541400
C	2.08413200	6.39207200	-2.15692100
H	0.42337500	7.39646900	-1.22466500
H	3.59001600	5.10892900	-3.00691800
S	1.18748500	-0.88456000	0.15291000
H	1.93550900	-9.13296500	2.83770300
H	2.58881100	7.30921000	-2.43756100

$T_{CT-Phen}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.62909600	-4.29615400	1.25990800
C	-2.19002100	-3.10405200	0.90321300
C	-1.40260300	-1.97141400	0.54841700
C	0.03912100	-2.13907200	0.63762500
C	0.59157100	-3.36046200	0.98445700
C	-0.18506600	-4.49353700	1.28798500
C	0.12253200	0.46795900	-0.18910500
C	-1.30434800	0.36619700	-0.25204100
C	-2.00351100	1.51180400	-0.71785100
H	-3.08075900	1.47925100	-0.79031600
C	-1.34745900	2.65504400	-1.09684200
C	0.76971700	1.64093500	-0.58513800
H	-2.28981400	-5.11939800	1.49258500
H	-3.26750700	-3.02402200	0.87508200
H	1.67153500	-3.41683700	1.05362000
H	-1.93384200	3.48490700	-1.46981500
H	1.84966100	1.67703600	-0.49726900
N	-1.98392400	-0.78322400	0.12414200
C	0.41041300	-5.77315100	1.62707100
C	-0.34644300	-6.80465000	2.24516400
C	1.77632300	-6.06386300	1.36193400
C	0.22558000	-8.02443200	2.58160900
H	-1.38741000	-6.63867000	2.49074900
C	2.33897800	-7.28413800	1.69972300
H	2.39595000	-5.33193300	0.85851800
C	1.57253800	-8.28183400	2.31537100
H	-0.38540100	-8.78187500	3.06135500
H	3.38370500	-7.46813200	1.47232700

C	0.07670600	2.75634200	-1.05156000
C	-3.43527600	-0.74665600	0.06171600
C	-4.17044500	-0.30216100	1.19678100
C	-4.06060100	-1.14528400	-1.09354000
C	-5.59948100	-0.27826800	1.09535000
C	-3.55887900	0.11217000	2.40928500
C	-5.47013400	-1.11778900	-1.18155100
H	-3.46601400	-1.47867700	-1.93545300
C	-6.21997400	-0.69352400	-0.11173700
C	-6.35759500	0.16220500	2.21301700
C	-4.32603900	0.53136100	3.46980000
H	-2.47966500	0.09479200	2.49428800
H	-5.95088900	-1.43340100	-2.09941000
H	-7.30226300	-0.67066500	-0.17567900
C	-5.73744300	0.55789300	3.37264200
H	-7.43893900	0.17976000	2.13294100
H	-3.84745200	0.84477400	4.39030600
H	-6.32646800	0.89179700	4.21884600
C	0.77712400	3.98250100	-1.47298600
C	0.15788500	5.24412500	-1.37172900
C	2.08745800	3.93999300	-1.98978700
C	0.81943200	6.40441500	-1.76107200
H	-0.84079900	5.32194500	-0.95885600
C	2.74722600	5.10117200	-2.37635600
H	2.58489400	2.98558100	-2.11622300
C	2.11864800	6.34266200	-2.26526100
H	0.32009000	7.36204700	-1.66283100
H	3.75256300	5.03573200	-2.77763300
S	1.13342000	-0.79343900	0.47158000
H	2.01500900	-9.23627100	2.57519600
H	2.63262300	7.24691200	-2.56998600

$T_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.60612300	-4.29919100	1.13980200
C	-2.16425000	-3.10916300	0.73499300
C	-1.36091500	-1.99004500	0.41686400
C	0.04427700	-2.15181300	0.52993200
C	0.59476700	-3.36839500	0.94311800
C	-0.20660600	-4.46242000	1.25493900
C	0.14711900	0.44456300	-0.29817100
C	-1.26835400	0.34946500	-0.32755000
C	-1.98138600	1.50139500	-0.73192000
H	-3.05807400	1.44945400	-0.77360300
C	-1.32957100	2.66165300	-1.07897600
C	0.79338400	1.63167900	-0.65425300
H	-2.26169000	-5.13410500	1.35116800
H	-3.23493900	-3.01412000	0.64380800
H	1.67097100	-3.44206700	1.04104500
H	-1.91849200	3.50981600	-1.40342600
H	1.87420400	1.66880300	-0.59405100
N	-1.96633200	-0.80201100	0.02096500
C	0.38334200	-5.74880200	1.68924900
C	-0.26726300	-6.54833600	2.64292100

C	1.60427400	-6.19843300	1.16075700
C	0.28868200	-7.75449100	3.05828300
H	-1.19979800	-6.21397000	3.08189600
C	2.15589100	-7.40719600	1.57371700
H	2.11231400	-5.61340300	0.40308600
C	1.50142600	-8.18923200	2.52500800
H	-0.22351200	-8.35227100	3.80331500
H	3.09404000	-7.74211700	1.14652300
C	0.08056800	2.75895900	-1.05127600
C	-3.42008700	-0.75980400	-0.02669700
C	-4.13199200	-0.36100400	1.13998500
C	-4.05664300	-1.12050000	-1.23863000
C	-5.57897200	-0.33414700	1.04526100
C	-3.52303700	0.00337800	2.36412500
C	-5.44070200	-1.08540500	-1.30151800
H	-3.45920100	-1.41595100	-2.09279700
C	-6.19868000	-0.70042800	-0.18544400
C	-6.31502300	0.05717200	2.18742200
C	-4.29546800	0.38633800	3.47638500
H	-2.44300900	-0.01172100	2.45092300
H	-5.94139700	-1.35898000	-2.22450500
H	-7.28146800	-0.67651400	-0.24645000
C	-5.68083400	0.41286000	3.38835500
H	-7.39843300	0.07799800	2.12012300
H	-3.79984000	0.66025000	4.40177500
H	-6.27749300	0.70805600	4.24533700
C	0.77136900	4.01143400	-1.43292100
C	0.20105100	5.26105700	-1.14074200
C	2.00977800	3.98031000	-2.09445900
C	0.85126300	6.43971600	-1.49344100
H	-0.74351700	5.31319200	-0.61244700
C	2.65582500	5.15992600	-2.45073200
H	2.45808000	3.02903100	-2.35600500
C	2.08017800	6.39417700	-2.15058200
H	0.39964900	7.39441600	-1.24983000
H	3.60607800	5.11486600	-2.97011200
S	1.18300400	-0.87197400	0.19306700
H	1.93228800	-9.13019000	2.84686500
H	2.58442100	7.31256700	-2.42789800

$T_{LE-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.53789000	-4.30618900	0.89231600
C	-2.16222900	-3.09231100	0.62821900
C	-1.46692200	-1.88010200	0.73509500
C	-0.11708200	-1.93893300	1.12406100
C	0.51141400	-3.15881400	1.34803500
C	-0.18526600	-4.37176500	1.24796500
C	-0.01097200	0.64111500	0.29152800
C	-1.37139300	0.46964700	-0.02035900
C	-1.97796700	1.44510800	-0.82352100
H	-3.02448100	1.35554100	-1.08040600
C	-1.25774000	2.53420900	-1.30135900
C	0.71239300	1.71165100	-0.22208800
H	-2.11309800	-5.21788200	0.78407200

H	-3.20301900	-3.09061400	0.33482200
H	1.55219400	-3.15746900	1.65028900
H	-1.76684800	3.25527800	-1.92958200
H	1.75782500	1.80699400	0.04714900
N	-2.10006100	-0.63956100	0.47488300
C	0.48916300	-5.66753400	1.50998400
C	-0.19018500	-6.71927000	2.14584400
C	1.82394800	-5.87851700	1.12831200
C	0.44099000	-7.93648000	2.38875300
H	-1.21379800	-6.57627500	2.47258400
C	2.45590000	-7.09474500	1.37413500
H	2.36543300	-5.09235900	0.61463900
C	1.76743900	-8.13031800	2.00491600
H	-0.10225300	-8.73157000	2.88718500
H	3.48524800	-7.23599600	1.06399200
C	0.10566800	2.68949500	-1.02361000
C	-3.52623100	-0.63335600	0.31933300
C	-4.34655000	-0.27438700	1.42480900
C	-4.11075300	-1.00202500	-0.96428600
C	-5.77938000	-0.28269800	1.24465200
C	-3.82069000	0.08832500	2.67995800
C	-5.46210500	-1.00534100	-1.11762500
H	-3.44686500	-1.27083900	-1.77678700
C	-6.31803600	-0.64453600	-0.01500700
C	-6.59749000	0.07251900	2.33469700
C	-4.68226400	0.44630900	3.77695500
H	-2.74755200	0.09819600	2.81929700
H	-5.90863600	-1.27889400	-2.06626600
H	-7.39332600	-0.64947500	-0.14828900
C	-6.03653900	0.43882000	3.60888600
H	-7.67409700	0.06889800	2.20748600
H	-4.23875200	0.71861700	4.72713900
H	-6.70120600	0.70516500	4.42210800
C	0.88187000	3.83955900	-1.55015300
C	0.30005100	5.11276400	-1.66122200
C	2.21827800	3.68659400	-1.95330600
C	1.02651600	6.19145200	-2.15876300
H	-0.72245700	5.26496100	-1.33526700
C	2.94555100	4.76614500	-2.44789400
H	2.68589900	2.71001800	-1.90062900
C	2.35324000	6.02398100	-2.55395200
H	0.55746400	7.16653000	-2.22899200
H	3.97410200	4.62167000	-2.75920500
S	0.77062900	-0.43363400	1.48168900
H	2.25900900	-9.07746700	2.19531600
H	2.91905500	6.86412000	-2.93995700

S18 Coordinates of the optimized geometries of molecule 4

S_0 geometry (Å) (B3LYP/6-311G(d,p))

C	-1.52356100	-4.34570800	0.79020500
C	-2.16501700	-3.14611400	0.50232300
C	-1.50953300	-1.91711100	0.65648500

C	-0.18184100	-1.94670100	1.11938100
C	0.46710000	-3.15151600	1.36546000
C	-0.19062400	-4.38089300	1.21706700
C	-0.07948600	0.63190900	0.29320900
C	-1.41611900	0.43467800	-0.09707500
C	-1.98501700	1.38931700	-0.95083900
H	-3.01117100	1.27950300	-1.27113400
C	-1.25273900	2.48372700	-1.39731100
C	0.65981200	1.70558700	-0.19044400
H	-2.06838600	-5.27063100	0.64349500
H	-3.18781300	-3.16921600	0.15454400
H	1.48963900	-3.12545200	1.72353500
H	-1.73290900	3.18831200	-2.06579100
H	1.68584300	1.81842300	0.13969500
N	-2.14957500	-0.68501700	0.36998700
C	0.50275100	-5.66153300	1.50289700
C	-0.18280200	-6.73900800	2.08684600
C	1.86246100	-5.83187300	1.19629100
C	0.46660300	-7.94187600	2.35209700
H	-1.22696200	-6.62768400	2.35572000
C	2.51244900	-7.03375600	1.46456400
H	2.41068600	-5.02508600	0.72336300
C	1.81768900	-8.09523700	2.04319600
H	-0.08228100	-8.75748800	2.80948000
H	3.56134200	-7.14350800	1.21265600
C	0.08868500	2.66437500	-1.03929800
C	-3.58375200	-0.66406700	0.25685900
C	-4.35414500	-0.26867300	1.39346900
C	-4.20577500	-1.01612900	-0.91935700
C	-5.78174100	-0.24536400	1.28611300
C	-3.76914800	0.10438300	2.63151200
C	-5.61265300	-0.99667700	-1.03521600
H	-3.60884700	-1.31364600	-1.77281400
C	-6.35491600	-0.61938200	0.04768300
C	-6.56813700	0.14365200	2.40004900
C	-4.55481000	0.47756100	3.69613500
H	-2.69086100	0.09011900	2.72389600
H	-6.10282500	-1.27334400	-1.95955300
C	-5.96408900	0.49808500	3.58187500
H	-7.64599900	0.15610500	2.30290000
H	-4.09108700	0.75949700	4.63431900
H	-6.56752000	0.79494200	4.43154400
C	0.87779700	3.82043500	-1.53258000
C	0.28353900	5.08209300	-1.69678500
C	2.23898800	3.68504600	-1.84980800
C	1.02213900	6.16666300	-2.16266300
H	-0.75959100	5.22107800	-1.43705900
C	2.97822500	4.77055700	-2.31260300
H	2.71809900	2.71728100	-1.75514000
C	2.37347300	6.01676900	-2.47217000
H	0.54272200	7.13269800	-2.27507200
H	4.02639600	4.63966700	-2.55732500
S	0.64267800	-0.42146800	1.53838300
F	-7.70557300	-0.59653900	-0.05129300

H	2.32334800	-9.03122300	2.25105200
H	2.94867100	6.86150500	-2.83346000

$S_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.60582700	-4.28823300	1.17780100
C	-2.16488600	-3.09877900	0.77288700
C	-1.36145500	-1.98797400	0.42735400
C	0.04468100	-2.15679800	0.51629400
C	0.59611400	-3.37374500	0.92713900
C	-0.20521900	-4.46025500	1.26389900
C	0.14712600	0.43966200	-0.31226700
C	-1.26912100	0.35205300	-0.31901400
C	-1.98241200	1.51226300	-0.69837300
H	-3.05996100	1.46896500	-0.72174000
C	-1.33002600	2.67218600	-1.04514300
C	0.79394500	1.62597500	-0.66984900
H	-2.26231700	-5.11620800	1.41216300
H	-3.23675500	-2.99998900	0.70306200
H	1.67365700	-3.45330200	1.00309700
H	-1.92006600	3.52731700	-1.34843000
H	1.87588100	1.65572700	-0.62935300
N	-1.96562500	-0.80233500	0.02241800
C	0.38523300	-5.74744800	1.69472500
C	-0.25065800	-6.53649600	2.66691000
C	1.59217500	-6.20832700	1.14419100
C	0.30609300	-7.74346800	3.07868900
H	-1.17177500	-6.19333100	3.12286900
C	2.14448500	-7.41792700	1.55367200
H	2.08810800	-5.63154700	0.37231500
C	1.50479400	-8.18949000	2.52338800
H	-0.19437900	-8.33308400	3.83804000
H	3.07144000	-7.76173100	1.10946300
C	0.08104500	2.76099200	-1.04366400
C	-3.41930700	-0.76482800	-0.03982800
C	-4.14097400	-0.36479100	1.12241600
C	-4.04166900	-1.12902600	-1.25314600
C	-5.58643000	-0.33980100	1.02497500
C	-3.54663300	0.00467100	2.34964800
C	-5.42534400	-1.10150400	-1.33472500
H	-3.44011600	-1.42449500	-2.10343600
C	-6.15441500	-0.71398000	-0.21206900
C	-6.34917400	0.05028900	2.15071200
C	-4.33614800	0.38858000	3.45492600
H	-2.46806400	-0.00620200	2.44672200
H	-5.94596300	-1.37251000	-2.24472700
C	-5.71859100	0.41028800	3.35423900
H	-7.42830700	0.06649600	2.06980500
H	-3.85094400	0.66667900	4.38421600
H	-6.32252000	0.70610800	4.20571000
C	0.77216600	4.01260400	-1.42711800
C	0.21325900	5.26310000	-1.11701100
C	2.00010200	3.97976000	-2.10790700
C	0.86439400	6.44078400	-1.47112700

H	-0.72266700	5.31666800	-0.57371600
C	2.64706300	5.15845900	-2.46538700
H	2.43916900	3.02813400	-2.38341800
C	2.08283400	6.39350800	-2.14738700
H	0.42180800	7.39605400	-1.21362400
H	3.58897200	5.11214600	-2.99962600
S	1.18428000	-0.88851600	0.14236800
F	-7.53121000	-0.69136600	-0.30733100
H	1.93618300	-9.13114400	2.84247500
H	2.58778000	7.31121000	-2.42567800

$S_{CT-Phen}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.60591300	-4.28826100	1.17799500
C	-2.16498600	-3.09869500	0.77342300
C	-1.36157100	-1.98792100	0.42778600
C	0.04456200	-2.15687200	0.51628100
C	0.59601700	-3.37396500	0.92670000
C	-0.20529800	-4.46045000	1.26356800
C	0.14701600	0.43956700	-0.31229300
C	-1.26922900	0.35207100	-0.31871000
C	-1.98250800	1.51228300	-0.69805900
H	-3.06006900	1.46905500	-0.72121100
C	-1.33011500	2.67212700	-1.04508100
C	0.79384800	1.62578800	-0.67018900
H	-2.26244400	-5.11617700	1.41245800
H	-3.23687000	-2.99980200	0.70393600
H	1.67358500	-3.45364200	1.00220700
H	-1.92018700	3.52725500	-1.34831900
H	1.87580300	1.65541700	-0.63001700
N	-1.96575700	-0.80221000	0.02301800
C	0.38518000	-5.74778600	1.69391600
C	-0.25048000	-6.53701600	2.66610100
C	1.59191600	-6.20863600	1.14291500
C	0.30629400	-7.74413400	3.07742800
H	-1.17143300	-6.19390700	3.12243100
C	2.14425600	-7.41837500	1.55194700
H	2.08767800	-5.63173700	0.37101700
C	1.50479500	-8.19012300	2.52166900
H	-0.19401500	-8.33388600	3.83678000
H	3.07105600	-7.76213300	1.10737800
C	0.08096200	2.76083300	-1.04393100
C	-3.41944300	-0.76454800	-0.03885700
C	-4.14077400	-0.36427900	1.12353200
C	-4.04215900	-1.12881300	-1.25195400
C	-5.58627300	-0.33914900	1.02640100
C	-3.54610300	0.00525900	2.35053700
C	-5.42583300	-1.10116600	-1.33323800
H	-3.44079000	-1.42446000	-2.10231800
C	-6.15458400	-0.71340100	-0.21041100
C	-6.34869300	0.05117600	2.15231600
C	-4.33529800	0.38941000	3.45599200
H	-2.46751100	-0.00571400	2.44736300
H	-5.94673300	-1.37222700	-2.24305800

C	-5.71776100	0.41124800	3.35561100
H	-7.42784400	0.06750100	2.07169400
H	-3.84981300	0.66757100	4.38511200
H	-6.32146900	0.70724200	4.20718400
C	0.77208300	4.01235400	-1.42764700
C	0.21335300	5.26290700	-1.11746300
C	1.99982600	3.97938900	-2.10877100
C	0.86447900	6.44052900	-1.47181300
H	-0.72242100	5.31658700	-0.57391600
C	2.64677600	5.15802200	-2.46649300
H	2.43876200	3.02772500	-2.38436600
C	2.08273300	6.39313300	-2.14839900
H	0.42201400	7.39583600	-1.21423700
H	3.58853500	5.11159600	-3.00098500
S	1.18418400	-0.88859000	0.14239300
F	-7.53139000	-0.69065400	-0.30538000
H	1.93620700	-9.13188500	2.84040600
H	2.58767400	7.31078000	-2.42688000

$T_{CT-Phen}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.63057600	-4.30987700	1.17523700
C	-2.19309600	-3.11731900	0.80373400
C	-1.40480300	-1.97545200	0.49350700
C	0.02811600	-2.13147100	0.61564900
C	0.57975100	-3.35389400	0.98427700
C	-0.19986900	-4.48278200	1.26541700
C	0.13044900	0.47656400	-0.21822900
C	-1.31179400	0.38192200	-0.25988400
C	-2.00931100	1.54495800	-0.68629200
H	-3.08866200	1.52539000	-0.73160900
C	-1.35444200	2.68828200	-1.06204400
C	0.77646500	1.64329000	-0.61468400
H	-2.28733600	-5.14751300	1.36773400
H	-3.26903100	-3.05079600	0.73026500
H	1.65770900	-3.40868500	1.08295400
H	-1.94492800	3.52707000	-1.40542100
H	1.85769600	1.66795700	-0.54266500
N	-1.98816200	-0.77858100	0.09582200
C	0.39916400	-5.76416000	1.64085600
C	-0.33911400	-6.73941700	2.35139700
C	1.73781900	-6.08486900	1.31315800
C	0.23081700	-7.95268000	2.71912800
H	-1.36113600	-6.53432100	2.64467900
C	2.30239700	-7.29800100	1.68243900
H	2.33358400	-5.38709200	0.73713100
C	1.55556600	-8.24493600	2.38996900
H	-0.36195700	-8.67316300	3.27226500
H	3.32906900	-7.51354900	1.40705800
C	0.08582400	2.77776700	-1.05721700
C	-3.43679400	-0.73934400	0.03937100
C	-4.17148700	-0.34081000	1.19309300
C	-4.06915100	-1.08756900	-1.12817600
C	-5.60023600	-0.31006000	1.10914300

C	-3.56024100	0.02696600	2.41975600
C	-5.47733400	-1.05971200	-1.21780700
H	-3.48242700	-1.38613300	-1.98785600
C	-6.19694600	-0.67932200	-0.12009600
C	-6.36407400	0.08190500	2.23771300
C	-4.32540700	0.40288200	3.49803200
H	-2.48088000	0.00885000	2.49920800
H	-5.98569500	-1.33225400	-2.13324400
C	-5.73656300	0.43115000	3.40846500
H	-7.44330900	0.10055200	2.15994900
H	-3.84367100	0.68103000	4.42801000
H	-6.32262100	0.73020900	4.26928200
C	0.78387700	3.99264800	-1.48224500
C	0.13901500	5.25116600	-1.47188800
C	2.12863800	3.96295700	-1.92004800
C	0.80304700	6.40750200	-1.86466800
H	-0.88378900	5.33034600	-1.12501200
C	2.78755100	5.12041900	-2.31170500
H	2.65423400	3.01764900	-1.98189600
C	2.13225700	6.35513900	-2.28770400
H	0.28069100	7.35757500	-1.83451700
H	3.81623700	5.05940400	-2.64995000
S	1.13152800	-0.79156500	0.44019900
F	-7.54758200	-0.64851500	-0.19411300
H	1.99735500	-9.19273000	2.67453000
H	2.64739600	7.25707200	-2.59695700

$T_{CT-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.53626000	-4.29208300	0.87065700
C	-2.16115100	-3.07852600	0.60645200
C	-1.46954100	-1.86570700	0.72538000
C	-0.12220500	-1.92231500	1.12153100
C	0.50730000	-3.14177000	1.34548200
C	-0.18636400	-4.35558900	1.23679400
C	-0.01720800	0.65800000	0.28971600
C	-1.37684300	0.48764100	-0.02581000
C	-1.98301400	1.46655900	-0.82454900
H	-3.03017200	1.38220900	-1.08039500
C	-1.26150900	2.55644400	-1.29902200
C	0.70704000	1.72972800	-0.22013700
H	-2.10823500	-5.20467400	0.75371500
H	-3.19938600	-3.07903900	0.30394200
H	1.54633800	-3.13946500	1.65355800
H	-1.77014500	3.28033600	-1.92428900
H	1.75192600	1.82449500	0.05128800
N	-2.10454900	-0.62425500	0.46696100
C	0.48882300	-5.65091800	1.49937100
C	-0.19294300	-6.70555900	2.12765600
C	1.82643500	-5.85817900	1.12585800
C	0.43888300	-7.92227100	2.37133600
H	-1.21898100	-6.56533300	2.44791600
C	2.45893300	-7.07398400	1.37231900
H	2.36984500	-5.06954400	0.61805900

C	1.76817400	-8.11252000	1.99565900
H	-0.10613400	-8.71977800	2.86390400
H	3.49053300	-7.21254100	1.06855400
C	0.10177600	2.70951400	-1.02035600
C	-3.52829800	-0.62369300	0.30816100
C	-4.35260500	-0.31019500	1.42560100
C	-4.10430700	-0.96322000	-0.98835100
C	-5.78567300	-0.33229300	1.25715700
C	-3.83227000	0.02574800	2.68980700
C	-5.45407100	-0.98477600	-1.14539900
H	-3.43925500	-1.20125000	-1.80837700
C	-6.28095600	-0.66694800	-0.02017200
C	-6.61768200	-0.02386500	2.34696500
C	-4.70001900	0.33673200	3.79526200
H	-2.75939600	0.05165000	2.82649200
H	-5.92577300	-1.23516800	-2.08706800
C	-6.05436000	0.31284400	3.62837700
H	-7.69166900	-0.04040000	2.21757700
H	-4.26097200	0.58815000	4.75307100
H	-6.72082300	0.54491400	4.45041500
C	0.87938500	3.86032100	-1.54331100
C	0.29907900	5.13449400	-1.65047900
C	2.21559800	3.70670200	-1.94667000
C	1.02704100	6.21375800	-2.14455300
H	-0.72326700	5.28700600	-1.32418000
C	2.94429400	4.78681300	-2.43792900
H	2.68192600	2.72936100	-1.89680300
C	2.35357000	6.04570100	-2.54012700
H	0.55931200	7.18966900	-2.21180400
H	3.97268300	4.64199500	-2.74957600
S	0.76181900	-0.41599300	1.48218700
F	-7.62157400	-0.69386800	-0.20745900
H	2.26021300	-9.05931100	2.18660100
H	2.92051300	6.88629300	-2.92347300

$T_{LE-Naph}$ geometry (Å) (B3LYP/6-311G(d,p))

C	-1.62981300	-4.29606500	1.26369600
C	-2.19145000	-3.10447400	0.90631900
C	-1.40484700	-1.97207200	0.54992900
C	0.03740000	-2.13884000	0.63865600
C	0.59054200	-3.35994100	0.98567200
C	-0.18526700	-4.49305200	1.29019000
C	0.11957400	0.46786100	-0.18892600
C	-1.30674000	0.36549700	-0.25434400
C	-2.00565300	1.50956200	-0.72336000
H	-3.08269800	1.47673600	-0.79843600
C	-1.34950300	2.65291000	-1.10246600
C	0.76693900	1.64099900	-0.58515900
H	-2.29006400	-5.11914000	1.49810600
H	-3.26903300	-3.02550600	0.87928900
H	1.67057200	-3.41573600	1.05420600
H	-1.93560500	3.48191200	-1.47777200
H	1.84672000	1.67776200	-0.49563800

N	-1.98660800	-0.78457500	0.12228200
C	0.41075300	-5.77238400	1.62894100
C	-0.34551900	-6.80410300	2.24736100
C	1.77667200	-6.06252900	1.36321000
C	0.22714600	-8.02360800	2.58372300
H	-1.38647600	-6.63861100	2.49324000
C	2.33993600	-7.28250400	1.70091800
H	2.39577000	-5.33042300	0.85941700
C	1.57408600	-8.28040200	2.31699200
H	-0.38332600	-8.78129500	3.06370400
H	3.38462700	-7.46614800	1.47313100
C	0.07414800	2.75509300	-1.05415300
C	-3.43566400	-0.74937700	0.05732500
C	-4.17487200	-0.30318800	1.19018000
C	-4.06120200	-1.15070200	-1.09664900
C	-5.60323600	-0.27672500	1.09760200
C	-3.56955400	0.11465200	2.40363500
C	-5.46874500	-1.12720800	-1.19405200
H	-3.47015900	-1.48625700	-1.93952200
C	-6.19367100	-0.69906000	-0.11733900
C	-6.37268000	0.16241900	2.20486600
C	-4.34032700	0.53501900	3.46140500
H	-2.49071400	0.09856600	2.49048700
H	-5.97257300	-1.43925800	-2.09928400
C	-5.75097100	0.56027800	3.36307000
H	-7.45148700	0.17765300	2.12093700
H	-3.86340100	0.85064300	4.38181300
H	-6.34131700	0.89513000	4.20761200
C	0.77468700	3.98142800	-1.47591900
C	0.15577000	5.24293700	-1.37363600
C	2.08436300	3.93839600	-1.99386400
C	0.81728600	6.40318200	-1.76327800
H	-0.84255500	5.32072700	-0.95986300
C	2.74415000	5.09951200	-2.38078400
H	2.58124900	2.98377300	-2.12088500
C	2.11597100	6.34104500	-2.26869900
H	0.31837100	7.36094900	-1.66435200
H	3.74908200	5.03394300	-2.78301900
S	1.13044000	-0.79250300	0.47340600
F	-7.54366700	-0.67144300	-0.19948500
H	2.01704700	-9.23463300	2.57672200
H	2.62992500	7.24522900	-2.57366100

S19 Coordinates of the optimized geometries of molecule 5

S_0 geometry (Å) (B3LYP/6-311G(d,p))

N	-4.94538600	0.26004500	0.07570100
N	4.94547900	0.25983700	-0.07582500
O	-0.00064400	-4.17885400	0.00005300
O	0.00014400	4.31651700	0.00022000
C	0.02019000	-2.18293300	1.26947300
C	0.03992500	-2.90120100	2.47826900
H	0.03949100	-3.98255500	2.42266800

C	0.05872600	-2.23950100	3.69211100
H	0.07382700	-2.79789300	4.62089300
C	0.05798300	-0.83995900	3.70928200
C	0.03896000	-0.12492200	2.52126800
H	0.03875400	0.95824600	2.54880700
C	0.01992900	-0.78180600	1.28325800
C	0.00004800	0.06304700	0.00003200
C	-0.01990500	-0.78181100	-1.28317700
C	-0.02061400	-2.18293000	-1.26938700
C	-0.00037000	-2.95442800	0.00004900
C	-0.04049300	-2.90121400	-2.47817600
H	-0.04039600	-3.98256500	-2.42254500
C	-0.05900000	-2.23952500	-3.69202200
H	-0.07421200	-2.79791300	-4.62080600
C	-0.05780100	-0.83997800	-3.70920700
C	-0.03863100	-0.12493400	-2.52120700
H	-0.03805700	0.95823400	-2.54875400
C	-1.28962900	0.91272400	0.01919400
C	-2.51136000	0.24640800	0.04175500
H	-2.50265700	-0.83364600	0.06062800
C	-3.74524800	0.93308100	0.06007000
C	-3.69043900	2.35345200	0.05995000
H	-4.59868700	2.93894200	0.05671700
C	-2.47953200	3.00684400	0.04365600
H	-2.44110900	4.08943100	0.03879500
C	-1.25643900	2.31448500	0.02159700
C	0.00010900	3.08487200	0.00012200
C	1.25662100	2.31442100	-0.02146900
C	1.28974200	0.91266700	-0.01912700
C	2.51144500	0.24628700	-0.04174400
H	2.50267700	-0.83376600	-0.06064000
C	3.74536000	0.93290500	-0.06009400
C	3.69061700	2.35328000	-0.05993600
H	4.59890500	2.93871500	-0.05673600
C	2.47974900	3.00673100	-0.04355300
H	2.44136600	4.08932000	-0.03862300
C	-5.01791900	-1.19706500	-0.04016400
H	-5.97114500	-1.43775700	-0.51831100
H	-4.24465600	-1.54456600	-0.72868100
C	-4.91469400	-1.93390900	1.30037100
H	-3.96370800	-1.72814400	1.79568800
H	-4.99252300	-3.01388000	1.14597200
H	-5.71886800	-1.62983200	1.97571000
C	-6.22274600	0.96054900	0.21284000
H	-6.91483000	0.27899100	0.71451100
H	-6.10063100	1.80970900	0.88864800
C	-6.82760600	1.41741200	-1.11983400
H	-6.16794500	2.11811800	-1.63594500
H	-7.78853100	1.91212100	-0.95107700
H	-6.99797800	0.56562600	-1.78345200
C	5.01798200	-1.19726500	0.04009700
H	5.97128700	-1.43796200	0.51808300
H	4.24482600	-1.54471600	0.72876800
C	4.91451500	-1.93418700	-1.30038700

H	3.96378200	-1.72779200	-1.79592000
H	4.99154600	-3.01419300	-1.14584300
H	5.71905200	-1.63076800	-1.97559400
C	6.22283400	0.96029200	-0.21318900
H	6.10059400	1.80951800	-0.88887900
H	6.91478200	0.27876700	-0.71510300
C	6.82802700	1.41701300	1.11938000
H	6.16875400	2.11809900	1.63547600
H	7.78917700	1.91123700	0.95048300
H	6.99804400	0.56522300	1.78308400
H	0.07251200	-0.30811000	4.65404700
H	-0.07210400	-0.30813700	-4.65398100

S_{CT} geometry (Å) (B3LYP/6-311G(d,p))

N	-5.01067100	0.05067000	0.08498200
N	4.80229500	0.49836400	-0.05979600
O	1.30641300	-3.99272500	-0.04673200
O	-0.26114100	4.31173500	-0.00594300
C	0.46346800	-2.15752100	1.22026700
C	0.61467100	-2.86338200	2.43953000
H	0.97592700	-3.88212800	2.37206200
C	0.30680200	-2.28092000	3.65659500
H	0.42981400	-2.84943200	4.57332000
C	-0.16658500	-0.96508900	3.70819800
C	-0.31603300	-0.25321400	2.51453500
H	-0.67640300	0.76934300	2.55678400
C	-0.00970200	-0.82296700	1.28080100
C	-0.09422100	0.04458700	-0.00223900
C	-0.04544100	-0.80712400	-1.29803800
C	0.42933000	-2.14200900	-1.26673300
C	0.79000800	-2.83279300	-0.03221600
C	0.54563100	-2.83325000	-2.49809600
H	0.90852700	-3.85253600	-2.45283400
C	0.20256900	-2.23666500	-3.69900900
H	0.29893600	-2.79444500	-4.62545900
C	-0.27277900	-0.92087100	-3.72122100
C	-0.38770900	-0.22323800	-2.51563700
H	-0.75036600	0.79914000	-2.53569100
C	-1.39993700	0.84603600	0.01911000
C	-2.58820900	0.13553700	0.04090700
H	-2.52672000	-0.94166000	0.05463700
C	-3.85255000	0.77228800	0.06592900
C	-3.86961200	2.20157000	0.06807500
H	-4.80480600	2.74185900	0.06934900
C	-2.69418700	2.90344600	0.04626000
H	-2.70002200	3.98633100	0.04034000
C	-1.43870600	2.25544800	0.02188100
C	-0.23123000	3.08264000	-0.00264600
C	1.06565600	2.35862300	-0.02255900
C	1.14413000	0.95367400	-0.01512000
C	2.39491200	0.36016600	-0.02593000
H	2.44531200	-0.71582000	-0.03297400
C	3.59354400	1.12021800	-0.05085000

C	3.48839200	2.54825400	-0.06444300
H	4.37043800	3.17072900	-0.06850300
C	2.25165600	3.13050600	-0.04661800
H	2.14323000	4.20743800	-0.04565500
C	-5.01941300	-1.41569300	-0.01482100
H	-5.96126300	-1.69480700	-0.49248400
H	-4.22817400	-1.73441500	-0.69349000
C	-4.89202800	-2.11871400	1.34036800
H	-3.94728300	-1.87458000	1.82902600
H	-4.93230900	-3.20167300	1.20017500
H	-5.70750300	-1.83231500	2.00957500
C	-6.32650000	0.68599600	0.21965400
H	-6.97441000	-0.02978200	0.73024400
H	-6.24603700	1.54767700	0.88344200
C	-6.95057500	1.08733200	-1.12116600
H	-6.33335400	1.82152000	-1.64283200
H	-7.93919200	1.52383100	-0.95646600
H	-7.06798800	0.21942800	-1.77439300
C	4.93849100	-0.96679400	0.05756600
H	5.90109000	-1.14848200	0.53818900
H	4.17417100	-1.34480200	0.73330700
C	4.87783800	-1.68316600	-1.29518000
H	3.91548600	-1.52991100	-1.78474000
H	5.00423400	-2.75518500	-1.13457200
H	5.66986900	-1.33776100	-1.96393600
C	6.06645000	1.23923100	-0.18845900
H	5.91535100	2.09502400	-0.84480200
H	6.76677900	0.57489200	-0.69698800
C	6.64053700	1.67373700	1.16444300
H	5.96545200	2.35805300	1.68124500
H	7.59445800	2.18177700	1.00718800
H	6.81661800	0.81329300	1.81310000
H	-0.41046900	-0.49805400	4.65519900
H	-0.54494800	-0.44313900	-4.65509100

T_{CT} geometry (Å) (B3LYP/6-311G(d,p))

N	-4.90575700	0.31121600	0.07315400
N	4.94209500	0.22919900	-0.07608700
O	-0.21443400	-4.21599700	0.00258600
O	0.05268200	4.32657100	0.00431800
C	-0.06703900	-2.20157000	1.25167300
C	-0.07211800	-2.91456400	2.47834600
H	-0.13812100	-3.99458500	2.43527500
C	0.00318400	-2.25277900	3.68982700
H	-0.00678700	-2.81955500	4.61506100
C	0.09157200	-0.85603100	3.72299100
C	0.09935000	-0.14562800	2.52356000
H	0.17080200	0.93677300	2.55153700
C	0.02167400	-0.78920900	1.28881900
C	0.01700600	0.06429500	0.00105000
C	-0.01505100	-0.78807300	-1.28702500
C	-0.10289600	-2.20055900	-1.24879600
C	-0.14494200	-2.92902000	0.00193300

C	-0.14296500	-2.91225800	-2.47561100
H	-0.20788200	-3.99227200	-2.43185500
C	-0.10184400	-2.24931500	-3.68804800
H	-0.13816000	-2.81517200	-4.61318700
C	-0.01461000	-0.85250100	-3.72234200
C	0.02729000	-0.14329100	-2.52286400
H	0.09766800	0.93915800	-2.55180400
C	-1.25550100	0.92828100	0.01902200
C	-2.48024400	0.27465400	0.03814900
H	-2.47716400	-0.80483800	0.05322200
C	-3.70947500	0.97628800	0.05880400
C	-3.65184600	2.40160400	0.06247500
H	-4.55726300	2.99067100	0.06141500
C	-2.43885900	3.04197900	0.04537700
H	-2.38753500	4.12375200	0.04154000
C	-1.21987500	2.33255200	0.02319400
C	0.04071500	3.09588200	0.00333600
C	1.28911500	2.31034200	-0.01820700
C	1.30223100	0.90469500	-0.01640500
C	2.51557900	0.23088600	-0.03787500
H	2.49300900	-0.84846700	-0.05466100
C	3.75548000	0.91144100	-0.05914700
C	3.72081000	2.33831000	-0.05994600
H	4.63611500	2.91198400	-0.05894800
C	2.51927800	2.99976100	-0.04026800
H	2.48619400	4.08220300	-0.03434200
C	-4.98819100	-1.15085400	-0.03453400
H	-5.94209200	-1.38082300	-0.51475000
H	-4.21251400	-1.50644800	-0.71341800
C	-4.89874200	-1.86883500	1.31662200
H	-3.94406500	-1.67467800	1.80836800
H	-4.99203700	-2.94763200	1.16880000
H	-5.70017000	-1.54662500	1.98637200
C	-6.18630800	1.01416400	0.20181500
H	-6.87559000	0.33282900	0.70570900
H	-6.06371000	1.86899900	0.86822100
C	-6.77979300	1.45262100	-1.14180500
H	-6.11986600	2.15263700	-1.65789500
H	-7.74380100	1.94264500	-0.98143300
H	-6.94118000	0.59386700	-1.79779400
C	5.00161100	-1.23389400	0.02824200
H	5.95284600	-1.48049500	0.50550300
H	4.22194800	-1.57819200	0.70855700
C	4.89705400	-1.94766500	-1.32411500
H	3.94535500	-1.73523800	-1.81416000
H	4.97170400	-3.02834600	-1.17906700
H	5.70296300	-1.63830100	-1.99454600
C	6.23306300	0.91235000	-0.20769600
H	6.12218300	1.76954100	-0.87313800
H	6.91011100	0.22100000	-0.71459500
C	6.83802200	1.34023100	1.13415700
H	6.19106500	2.05024800	1.65308700
H	7.80919500	1.81503000	0.97109600
H	6.98792100	0.47852600	1.78904500

H	0.15269200	-0.32797300	4.66745800
H	0.01940200	-0.32346800	-4.66763000

S20 Frequencies of all geometries of molecule 5 computed at (B3LYP/6-311G(d,p)) level of theory

molecule-3		
ω_{S_0}	$\omega_{S_{CT}}$	$\omega_{T_{CT}}$
11.11	14.76	10.52
21.63	25.21	12.58
29.42	25.94	28.70
29.94	31.69	29.15
35.18	36.08	35.76
56.08	53.84	56.08
56.99	56.94	56.57
57.97	62.22	61.71
61.75	65.73	63.96
75.78	75.10	75.59
84.56	84.64	85.51
87.90	89.31	87.70
100.00	104.49	105.19
114.30	114.66	114.21
115.03	120.35	118.26
119.56	127.69	125.72
125.31	135.51	127.73
129.69	148.26	140.86
169.35	165.40	168.10
181.89	185.63	181.53
202.23	197.04	202.03
215.80	209.24	214.49
217.02	215.16	216.85
218.03	219.45	218.76
221.43	219.57	222.30
237.63	239.03	236.67
241.93	241.80	237.08
260.18	259.51	258.69
270.76	276.61	273.06
281.50	281.11	276.97
287.68	287.65	284.65

molecule-3		
ω_{S_0}	$\omega_{S_{CT}}$	$\omega_{T_{CT}}$
295.90	288.70	291.84
307.18	310.66	308.70
341.21	322.72	320.12
343.17	341.42	341.86
343.53	343.62	342.16
350.28	345.69	346.53
370.33	369.36	372.25
377.28	383.23	377.35
414.67	395.77	383.44
424.85	427.66	424.08
426.98	431.14	430.42
427.37	440.68	434.78
460.21	452.28	453.51
461.59	466.80	460.80
469.94	474.52	473.21
481.99	485.58	482.87
484.10	486.58	483.53
507.42	513.72	504.94
527.91	535.51	528.47
540.81	545.38	537.47
545.30	555.04	547.85
559.36	566.01	550.78
582.04	579.48	575.26
584.11	582.02	577.34
586.10	590.17	586.32
642.56	626.34	587.65
644.66	636.70	631.97
645.50	641.12	634.14
654.33	648.99	647.44
680.46	649.89	649.30
682.38	666.59	672.76
697.33	676.89	676.43
711.03	698.12	696.35
712.40	707.01	708.25
725.66	712.80	712.14
744.63	741.85	739.47
751.65	744.88	744.06
774.03	747.21	748.47
782.62	757.15	759.56
787.08	772.55	770.21
788.69	780.72	770.74
793.32	788.58	785.56
795.43	794.57	793.02

molecule-3		
ω_{S_0}	$\omega_{S_{CT}}$	$\omega_{T_{CT}}$
797.06	798.81	798.23
801.10	804.07	799.21
821.46	808.49	802.96
831.47	824.69	817.45
841.32	828.12	827.15
852.28	852.00	849.26
855.70	872.43	864.00
863.63	875.29	866.07
889.03	882.39	867.76
903.64	887.81	879.48
916.89	900.39	896.83
917.57	900.66	912.67
928.35	914.80	921.94
930.27	930.30	925.14
941.70	931.40	932.03
944.09	932.71	932.32
946.20	932.95	940.50
953.09	936.73	941.61
991.49	947.20	944.64
991.84	950.93	948.43
998.84	987.78	981.60
1000.02	990.75	982.11
1001.89	996.70	997.50
1014.89	1006.23	1002.96
1015.47	1012.74	1005.59
1021.86	1015.27	1016.15
1038.48	1029.56	1032.55
1058.13	1049.31	1047.46
1067.28	1053.89	1059.84
1085.34	1071.94	1080.99
1085.35	1076.30	1081.22
1094.85	1082.04	1086.23
1094.98	1089.40	1087.58
1104.16	1098.58	1098.64
1112.28	1101.91	1103.64
1112.44	1108.80	1110.47
1112.85	1111.46	1110.84

molecule-3		
ω_{S_0}	$\omega_{S_{CT}}$	$\omega_{T_{CT}}$
1121.77	1119.53	1124.26
1135.01	1123.30	1128.19
1171.05	1130.28	1157.38
1172.05	1155.64	1157.90
1175.32	1167.22	1167.10
1180.87	1173.17	1174.01
1190.38	1175.21	1174.19
1192.72	1177.06	1175.97
1195.81	1187.96	1185.40
1202.57	1198.88	1195.58
1218.12	1200.32	1205.41
1218.29	1210.28	1209.86
1219.59	1212.65	1212.50
1231.41	1221.78	1227.91
1268.56	1256.84	1272.68
1283.55	1260.59	1273.57
1294.02	1278.78	1279.65
1299.94	1279.50	1289.71
1302.90	1288.02	1291.33
1314.16	1291.13	1295.32
1316.67	1315.05	1314.95
1319.69	1317.29	1315.95
1330.96	1320.75	1317.79
1340.24	1322.90	1323.43
1343.52	1327.94	1324.52
1353.64	1335.10	1333.46
1358.07	1362.07	1343.36
1364.23	1370.43	1360.71
1381.47	1373.05	1368.75
1382.64	1378.44	1377.69
1394.32	1381.12	1379.57
1395.36	1387.41	1385.46
1408.53	1410.06	1390.29
1408.56	1412.13	1408.75
1411.18	1412.57	1409.05
1411.22	1414.30	1411.51
1429.87	1422.50	1412.07
1434.77	1434.58	1428.87
1466.45	1437.75	1432.29
1467.09	1455.72	1445.42
1475.71	1466.58	1462.30
1479.05	1477.35	1463.33

molecule-3		
ω_{S_0}	$\omega_{S_{CT}}$	$\omega_{T_{CT}}$
1489.22	1485.70	1469.84
1489.23	1485.82	1485.17
1490.79	1488.30	1488.81
1490.87	1489.34	1489.19
1493.10	1489.72	1490.21
1493.43	1490.64	1490.41
1498.94	1493.10	1492.93
1499.07	1493.52	1493.28
1505.12	1497.94	1498.56
1511.63	1498.44	1498.68
1511.78	1513.55	1509.23
1514.66	1515.48	1512.98
1525.56	1516.41	1513.75
1526.65	1525.13	1522.72
1543.24	1531.64	1527.42
1548.11	1538.91	1537.23
1574.72	1541.27	1538.88
1582.69	1546.01	1551.50
1602.91	1554.92	1557.24
1620.18	1560.90	1564.41
1631.42	1585.61	1578.63
1638.45	1587.06	1598.62
1640.00	1614.42	1621.62
1640.32	1628.43	1625.04
1688.32	1636.77	1626.02
1712.85	1688.94	1685.05
3029.52	3034.72	3034.40
3029.55	3035.60	3034.78
3030.18	3042.64	3035.19
3030.21	3043.40	3035.47
3039.25	3055.80	3052.59
3039.27	3061.52	3052.89
3048.00	3072.61	3059.14
3048.16	3078.39	3059.71
3073.65	3090.35	3088.68
3073.65	3093.27	3089.12

molecule-3		
ω_{S_0}	$\omega_{S_{CT}}$	$\omega_{T_{CT}}$
3076.24	3103.90	3090.95
3076.25	3107.23	3091.70
3094.30	3108.39	3103.10
3094.32	3109.68	3103.37
3094.81	3114.08	3105.52
3094.85	3116.34	3106.29
3107.01	3119.24	3113.84
3107.03	3126.60	3114.29
3109.15	3129.31	3117.72
3109.23	3138.07	3118.31
3167.63	3148.19	3154.75
3167.69	3148.70	3154.79
3180.49	3157.28	3161.35
3180.65	3157.91	3161.55
3189.96	3179.99	3181.99
3190.35	3180.33	3182.08
3191.17	3191.31	3193.26
3191.37	3192.21	3193.54
3201.60	3195.98	3195.78
3202.03	3204.68	3196.00
3210.56	3220.31	3217.66
3211.01	3227.03	3218.00
3212.00	3230.60	3220.26
3212.31	3249.25	3221.29

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