

Electronic Supplementary Information: How a Linear Triazene Photoisomerizes in a Volume-conserving Fashion

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Unrelaxed COSMO-ADC(2) Torsion Potentials

Starting from the S_1 ADC(2)/SVP optimized structure, unrelaxed torsion potentials of the triazene group are calculated at PTED-COSMO-ADC(2)/SVP level, figure S1. This calculations show that the solvent effect has a small effect on the optimal values of the triazene torsion angles.

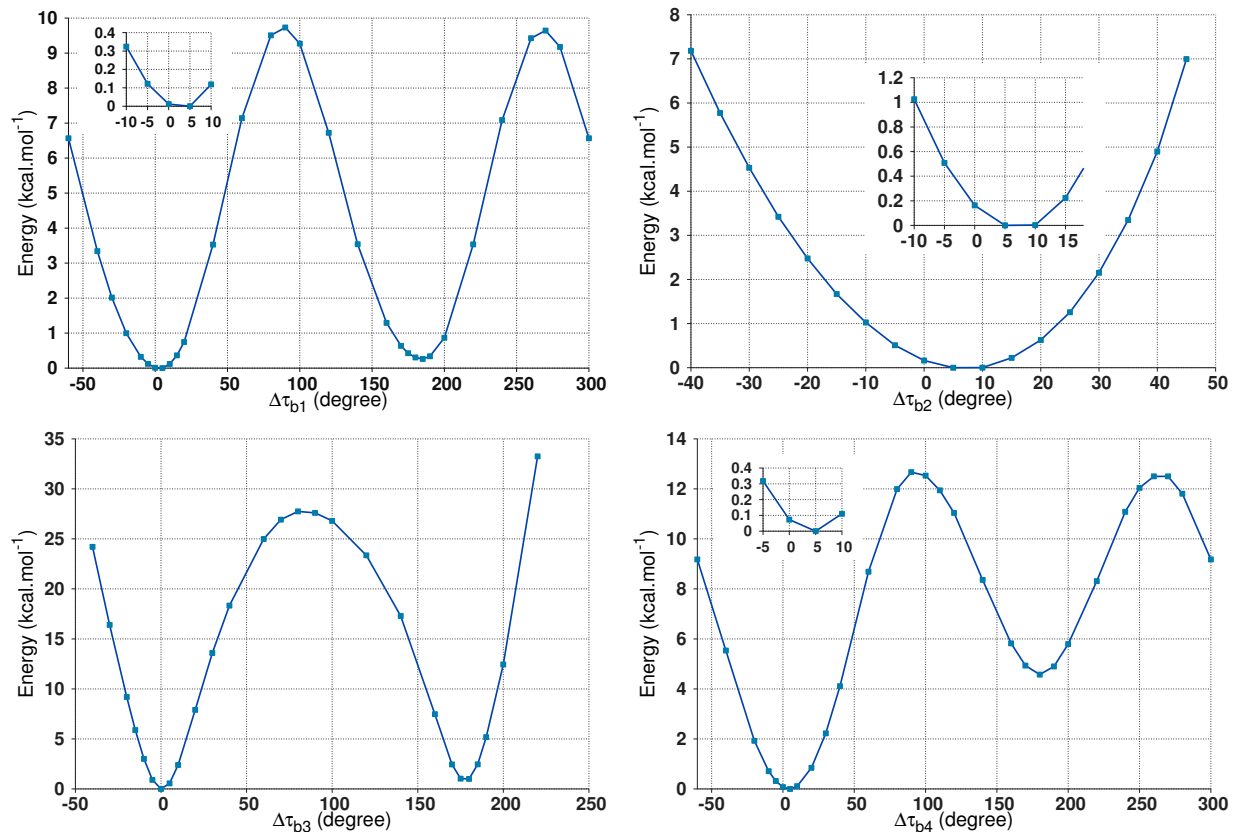


Figure S1: Unrelaxed torsion potential of the central torsion angles calculated at PTED-COSMO-ADC(2)/SVP level.

Natural Transition Orbitals of ET conformer

Table S1: Natural transition orbitals of the ET conformer calculated at the ADC(2)/SVP level in vacuum. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

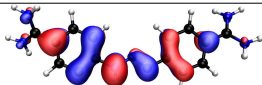
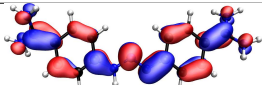
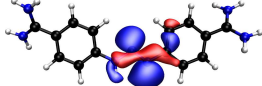
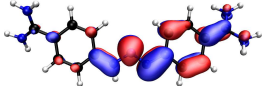
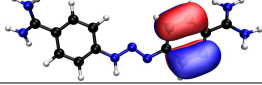
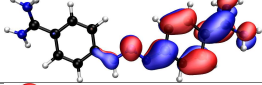
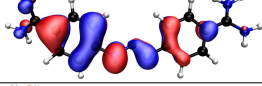
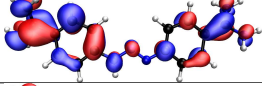
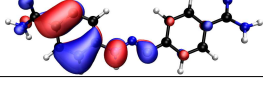
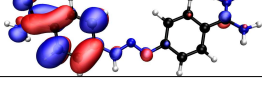
EEL	VEE	OS	OCC	VIR	Contrib.
ET ₁	3.54	1.30			95.0 %
ET ₂	3.73	0.01			99.7 %
ET ₃	4.61	0.00			72.0 %
ET ₄	4.65	0.09			83.6 %
ET ₅	4.75	0.02			57.5 %

Table S2: Natural transition orbitals of the ET conformer calculated at the ADC(2)/SVP level in COSMO. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

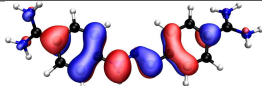
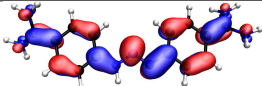
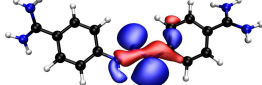
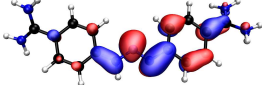
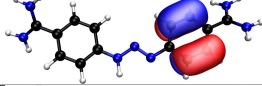

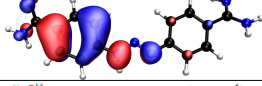
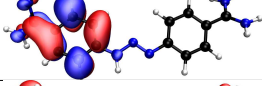
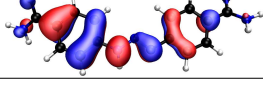
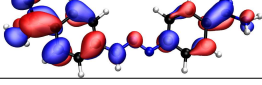
EEL	VEE	OS	OCC	VIR	Contrib.
ET ₁	3.52	1.28			96.2 %
ET ₂	3.87	0.00			99.7 %
ET ₃	4.66	0.01			70.6 %
ET ₄	4.77	0.02			62.3 %
ET ₅	4.92	0.12			86.2 %

Table S3: Natural transition orbitals of the ET conformer calculated at the ADC(2)/aug-cc-pVDZ level in vacuum. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

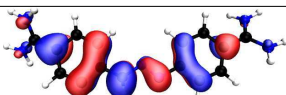
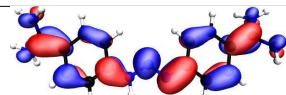
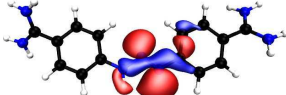
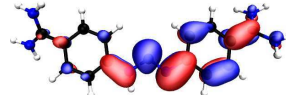
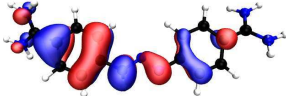
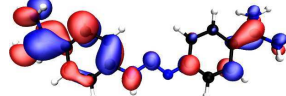
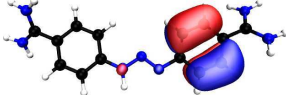
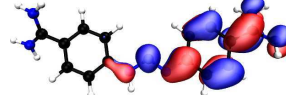
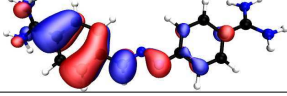
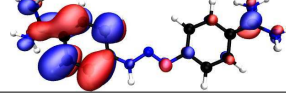
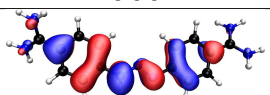
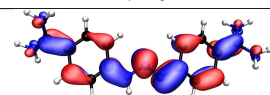
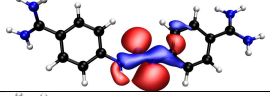
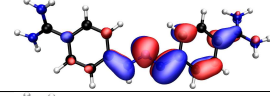
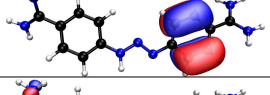
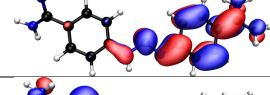
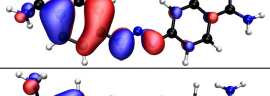
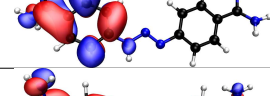
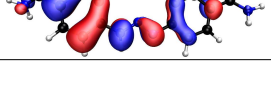
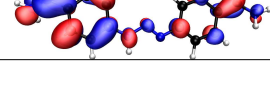
State	VEE	OS	OCC	VIR	Contrib.
S ₁	3.4	1.24			95.3 %
S ₂	3.7	0.00			99.7 %
S ₃	4.4	0.07			86.6 %
S ₄	4.5	0.03			73.8 %
S ₅	4.6	0.03			59.0 %

Table S4: Natural transition orbitals of the ET conformer calculated at the ADC(2)/aug-cc-pVDZ level in COSMO. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

EEL	VEE	OS	OCC	VIR	Contrib.
S ₁	3.32	1.17			96.5 %
S ₂	3.84	0.00			99.7 %
S ₃	4.53	0.01			64.5 %
S ₄	4.58	0.08			69.5 %
S ₅	4.74	0.09			79.0 %

Natural Transition Orbitals of EC conformer

Table S5: Natural transition orbitals of the EC conformer calculated at the ADC(2)/SVP level in vacuum. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

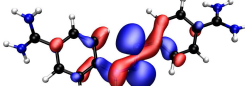
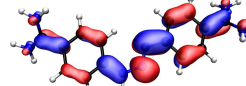
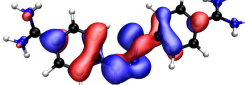
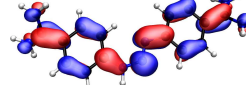
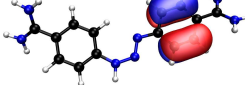
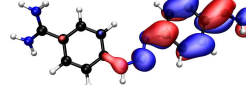
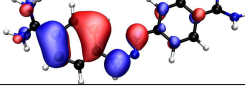
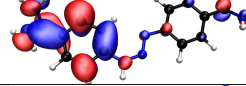
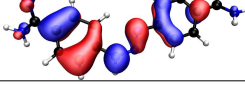
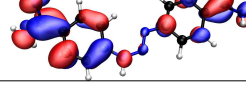
EEL	VEE	OS	OCC	VIR	Contrib.
EC ₁	3.60	0.29			96.5 %
EC ₂	3.65	0.92			93.5 %
EC ₃	4.64	0.02			74.7 %
EC ₄	4.73	0.04			63.7 %
EC ₅	4.77	0.05			71.5 %

Table S6: Natural transition orbitals of the EC conformer calculated at the ADC(2)/SVP level in COSMO. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

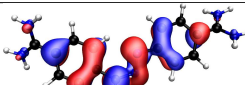
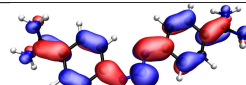
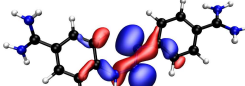
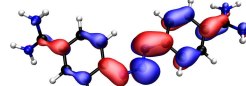
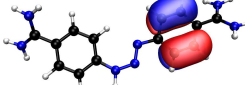
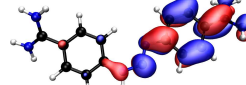
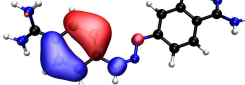
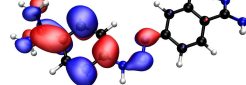
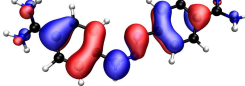
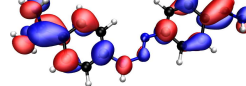
EEL	VEE	OS	OCC	VIR	Contrib.
S ₁	3.64	1.14			95.6 %
S ₂	3.74	0.08			98.8 %
S ₃	4.71	0.02			69.8 %
S ₄	4.78	0.00			55.5 %
S ₅	5.00	0.09			84.5 %

Table S7: Natural transition orbitals of the EC conformer calculated at the ADC(2)/aug-cc-pVDZ level in vacuum. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

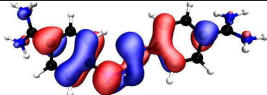
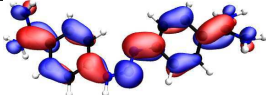
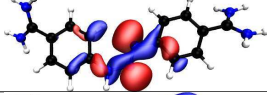
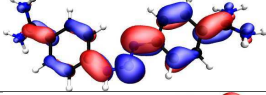
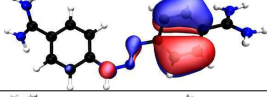
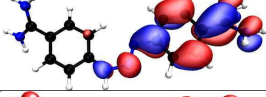
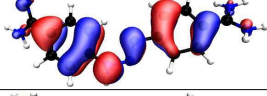
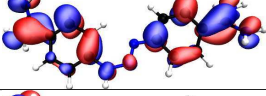
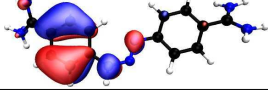
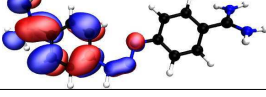
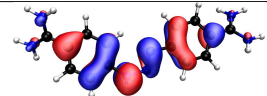
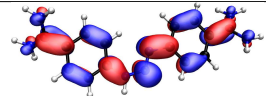
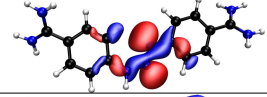
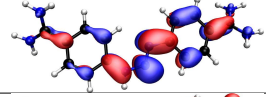
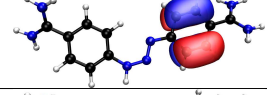
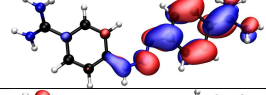
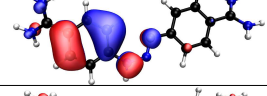
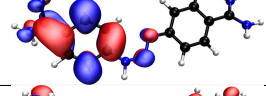
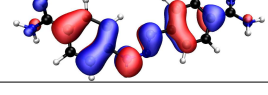
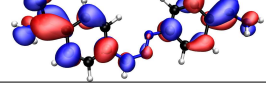
State	VEE	OS	OCC	VIR	Contrib.
S ₁	3.5	1.10			94.5 %
S ₂	3.6	0.08			98.5 %
S ₃	4.5	0.01			69.9 %
S ₄	4.5	0.09			74.8 %
S ₅	4.6	0.00			57.1 %

Table S8: Natural transition orbitals of the EC conformer calculated at the ADC(2)/aug-cc-pVDZ level in COSMO. The isosurfaces chosen to visualize orbitals are at +0.03 (blue) and -0.03 (red). VEEs are in eV and the contribution of each pair is shown in the last column.

EEL	VEE	OS	OCC	VIR	Contrib.
EC _{S1}	3.49	1.17			96.1 %
EC _{S2}	3.69	0.01			99.5 %
EC _{S3}	4.58	0.02			67.4 %
EC ₄	4.64	0.01			56.4 %
EC ₅	4.78	0.07			82.1 %

Supplementary Experimental Data

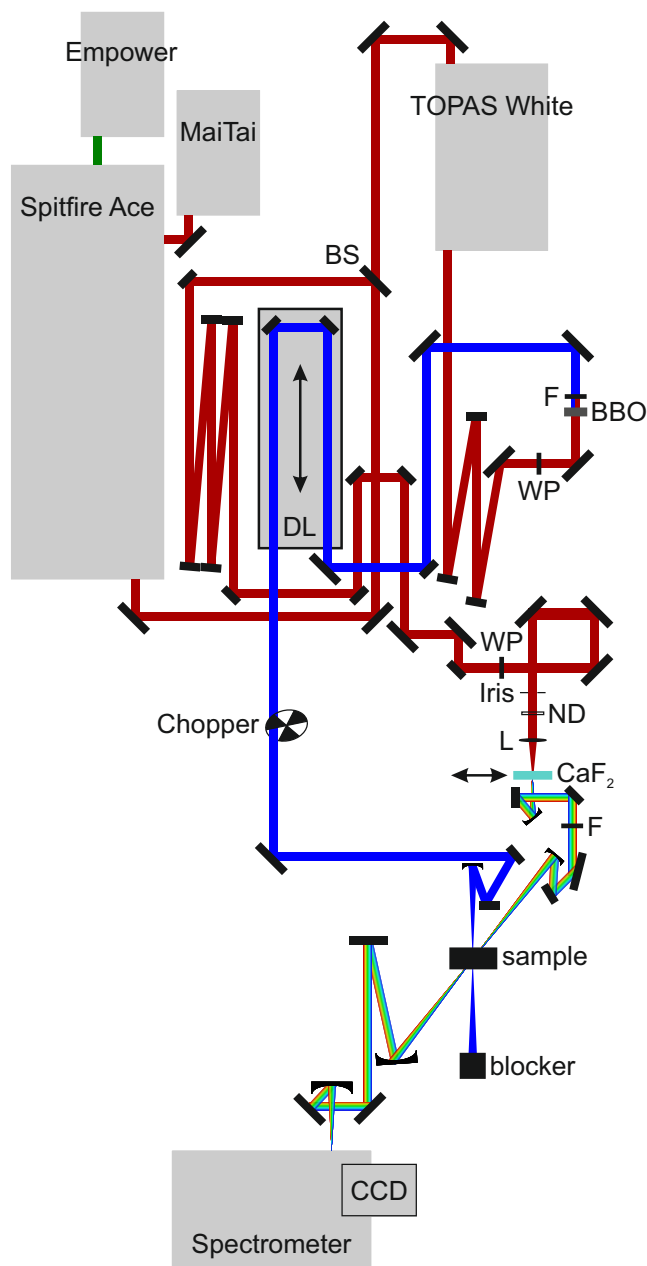


Figure S2: Sketch of the transient absorption setup with visible white-light probe. DL: delay line, F: filter, BS: beam splitter, BBO: β -barium borate crystal for the second harmonic generation, WP: half-wave plate, ND: neutral density filter, L: lens, CaF₂: calcium fluoride plate for the generation of the supercontinuum, CCD: charge-coupled device.

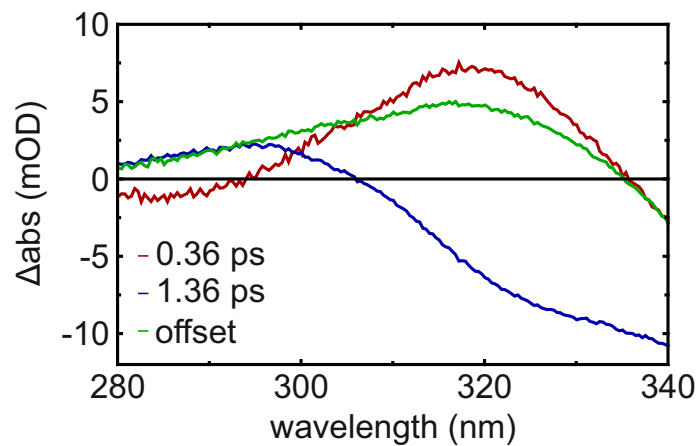


Figure S3: Decay associated spectra for berenil in 50 mM Tris-HCl and 25 mM CaCl₂ for the UV white-light probe.

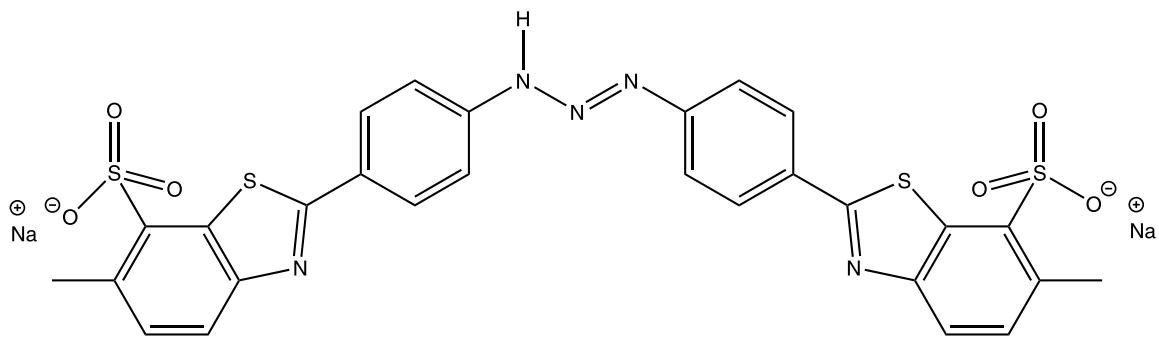


Figure S4: Chemical structure of thiazole yellow.

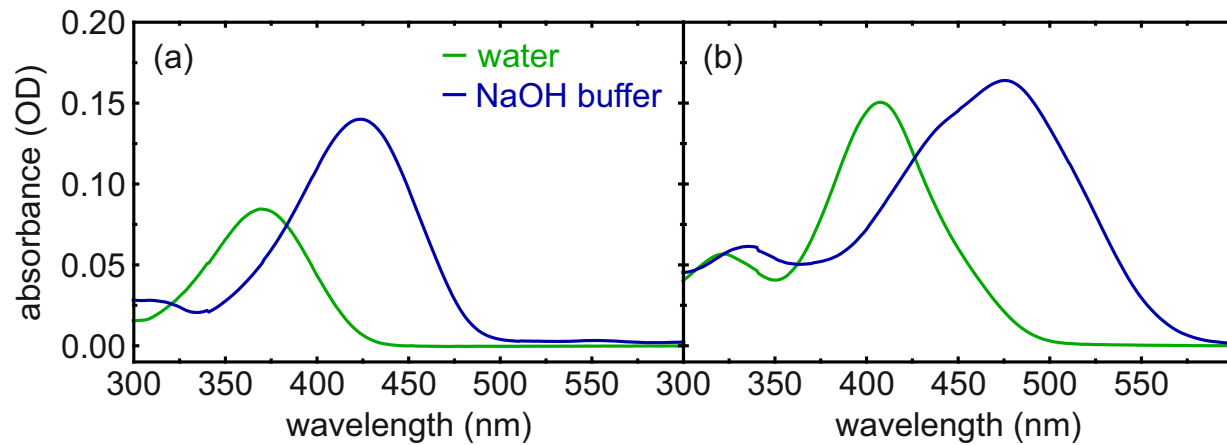


Figure S5: Absorption of a) berenil and b) thiazole yellow in water (green) and NaOH buffer, pH 13.5 (blue).

COSMO-ADC(2) Minimal Forcefield

Additive force-fields are built by assuming that degrees of freedom are decoupled and thus the changes of the (potential) energy of the system is equal to the sum of the changes in each degree of freedom, equation 1.

$$\Delta E = \sum_i \Delta E_i. \tag{1}$$

Therefore to have an analytical expression for the unrelaxed PES around a particular geometry, it is enough to interpolate the unrelaxed potential energy curves to have an analytical expression for each term of the equation 1. The interpolation of unrelaxed energy curves—calculated at the COSMO-ADC(2)/SVP level for changes in the τ_{b2} and τ_{b3} dihedral angles are done via a simple polynomial expansion (using 3 terms is sufficient for achieving quantitative convergence) around the ET_{S1} structure, equation 2.

$$\Delta E_{\tau_i}(\delta\tau_i) = a \cdot (\delta\tau_i - b)^2 + c \cdot (\delta\tau_i - b)^3 + d \cdot (\delta\tau_i - b)^4 \tag{2}$$

The two dimensional force-field parameters are listed in table S9.

Table S9: The minimal force-field parameters.

parameters	τ_{b2}	τ_{b3}
a	0.003661	0.028256
b	7.76111	0.53892
c	$2.48389 \cdot 10^{-5}$	$-3.91249 \cdot 10^{-5}$
d	$3.01446 \cdot 10^{-7}$	$-1.75301 \cdot 10^{-5}$

Equivalency of Clockwise and Anti-clockwise Deexcitation Pathways of ET Conformer

In this section, energy alleviation along different IRC pathways of the ET conformer on the excited state (IRC₂ and IRC₃) and on the ground state (IRC₄ and IRC₅) are compared.

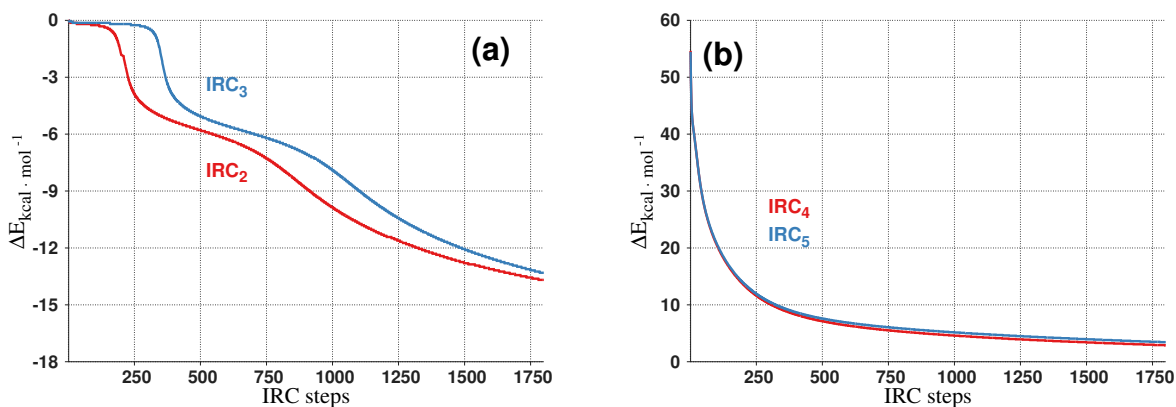


Figure S6: (a) The difference between the energy of the lowest excited state of the TS_{S1} geometry and the lowest excited state deexcitation pathways (IRC₂ and IRC₃), calculated at ADC(2)/SVP level of theory. (b) The difference between the ground state energy of the ET1 conformer and the ground state relaxation pathways (IRC₄ and IRC₅) of the ET conformer calculated at MP2/SVP level of theory.

NTOs of Ground State Transient Absorption

$ET_{S_0} \rightarrow ET_{S_1}$:

Table S10: Part I: VEE, OS and NTOs of $S_0 \rightarrow S_1$ excitation for selected IRC₅ steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

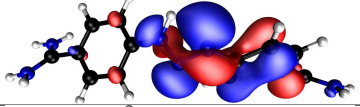
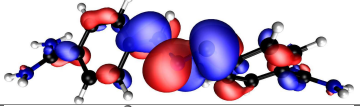
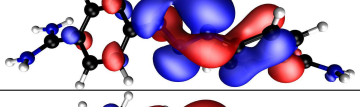
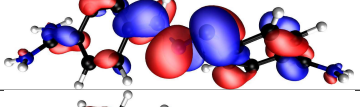
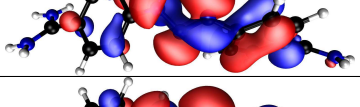
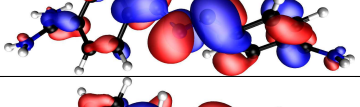
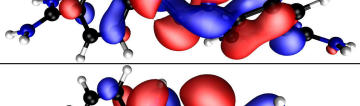
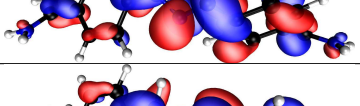
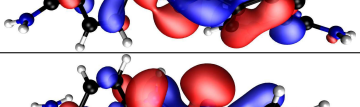
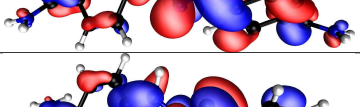
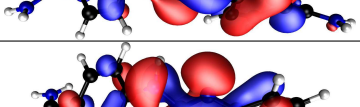
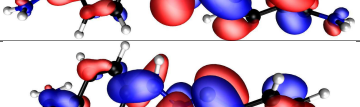
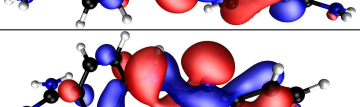
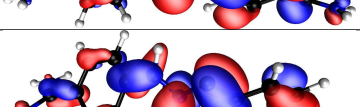
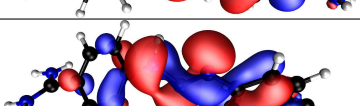
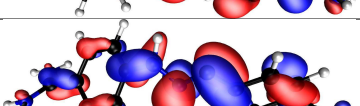
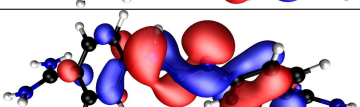
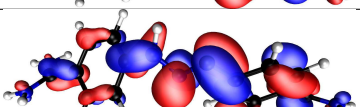


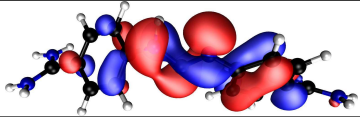
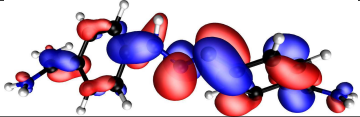
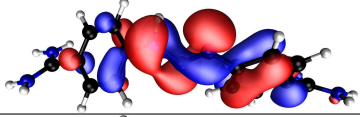
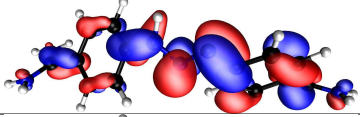
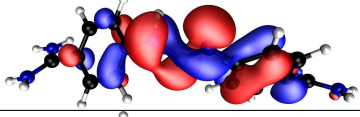
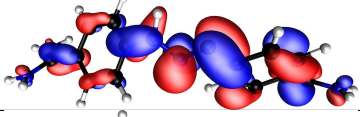
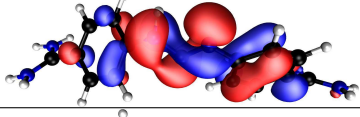
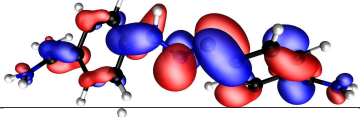
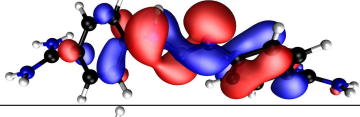
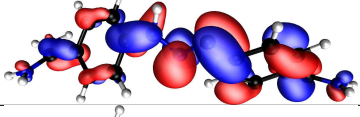
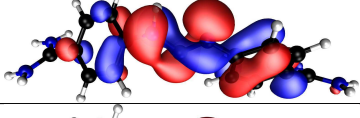
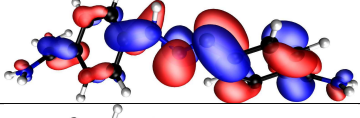
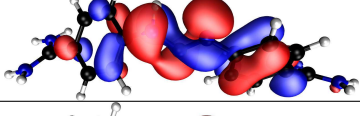
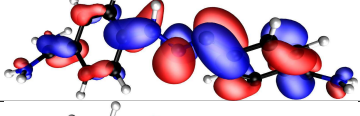
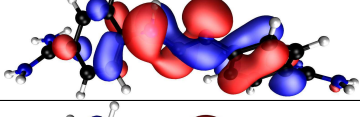
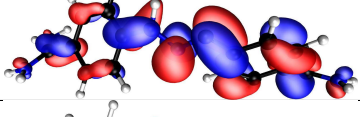
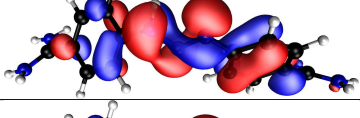
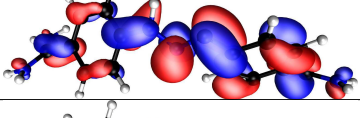
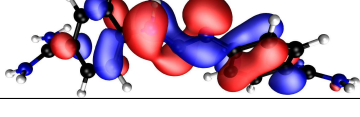
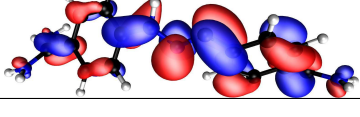
EEL	Step	VEE	OS	OCC	VIR	Contrib.
1	50	1.8	0.20			98.9 %
1	100	2.4	0.38			97.9 %
1	150	2.7	0.48			97.2 %
1	200	2.9	0.54			96.6 %
1	250	3.0	0.57			96.2 %
1	300	3.1	0.59			95.8 %
1	350	3.2	0.61			95.5 %
1	400	3.2	0.62			95.3 %
1	450	3.3	0.63			95.1 %
1	500	3.3	0.64			94.9 %

Table S11: Part II: VEE, OS and NTOs of $S_0 \rightarrow S_1$ excitation for selected IRC₅ steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

EEL	Step	VEE	OS	OCC	VIR	Contrib.
1	550	3.3	0.65			94.8 %
1	600	3.3	0.65			94.7 %
1	650	3.4	0.66			94.6 %
1	700	3.4	0.66			94.5 %
1	750	3.4	0.67			94.5 %
1	1000	3.4	0.69			94.3 %
1	1250	3.4	0.72			94.3 %
1	1500	3.4	0.73			94.3 %
1	1750	3.4	0.75			94.3 %
1	2000	3.4	0.77			94.3 %

$\text{ET}_{S_0} \rightarrow \text{ET}_{S_2}$:

Table S12: Part I: VEE, OS and NTOs of $S_0 \rightarrow S_2$ excitation for selected IRC_5 steps, calculated at $\text{ADC}(2)/\text{aTZ}$ level. The isosurfaces chosen to visualize orbitals are at $+0.03$ (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

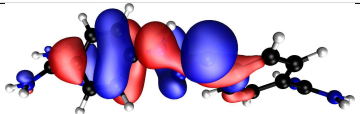

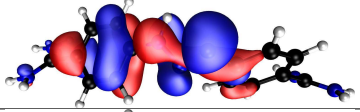
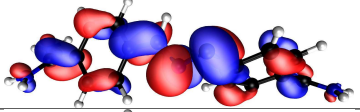
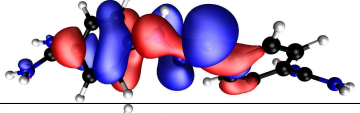
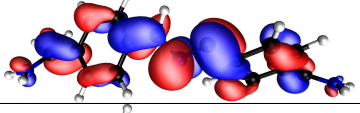
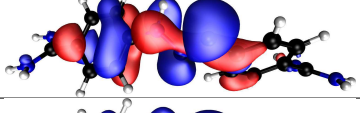
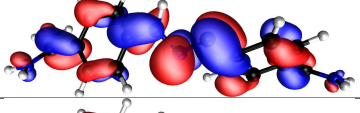
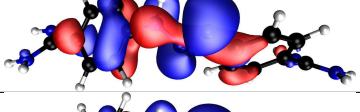
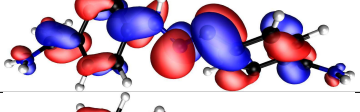
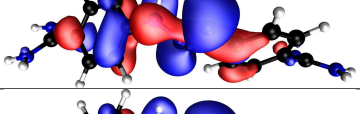
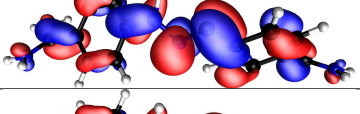
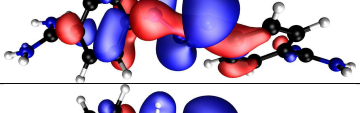
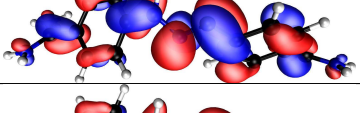
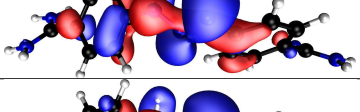
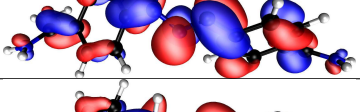
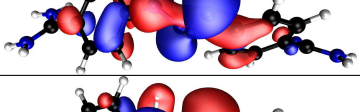
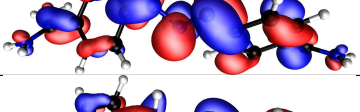
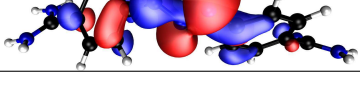
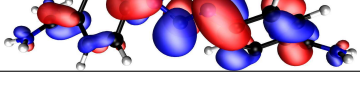
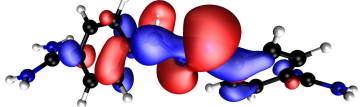
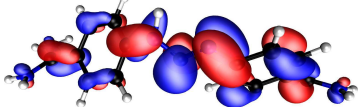
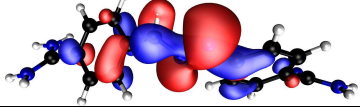
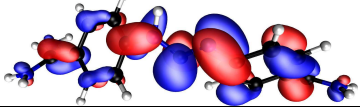
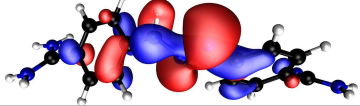
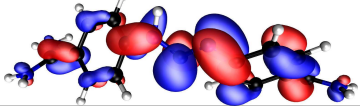
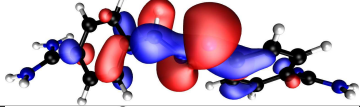
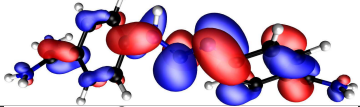
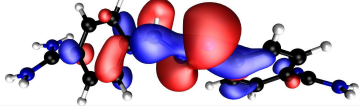
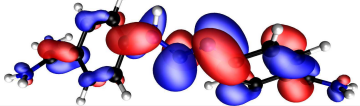
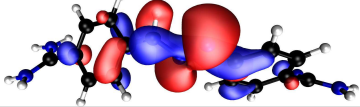
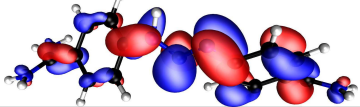
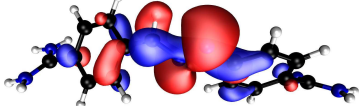
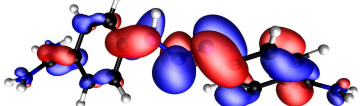
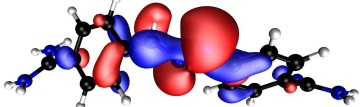
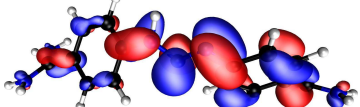
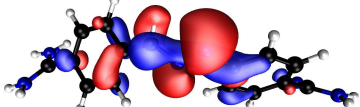
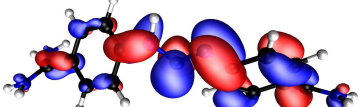
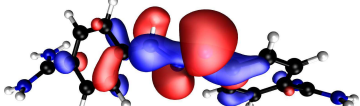
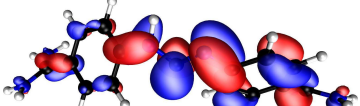
EEL	Step	VEE	OS	OCC	VIR	Contrib.
2	50	3.6	0.82			81.8 %
2	100	3.7	0.67			83.4 %
2	150	3.8	0.59			81.8 %
2	200	3.9	0.54			80.8 %
2	250	3.9	0.50			80.7 %
2	300	3.9	0.48			81.3 %
2	350	3.9	0.46			82.0 %
2	400	3.9	0.45			82.9 %
2	450	3.9	0.44			83.7 %
2	500	3.9	0.43			84.4 %

Table S13: Part II: VEE, OS and NTOs of $S_0 \rightarrow S_2$ excitation for selected IRC₅ steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

EEL	Step	VEE	OS	OCC	VIR	Contrib.
2	550	3.9	0.43			85.1 %
2	600	3.9	0.42			85.7 %
2	650	3.9	0.42			86.2 %
2	700	3.9	0.42			86.7 %
2	750	3.9	0.41			87.1 %
2	1000	3.9	0.40			88.7 %
2	1250	3.9	0.38			89.7 %
2	1500	3.9	0.37			90.5 %
2	1750	3.9	0.36			91.1 %
2	2000	3.9	0.35			91.6 %

$\text{ET}_{S_0} \rightarrow \text{ET}_{S_3}$:

Table S14: Part I: VEE, OS and NTOs of $S_0 \rightarrow S_3$ excitation for selected IRC_5 steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

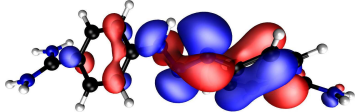
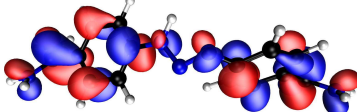
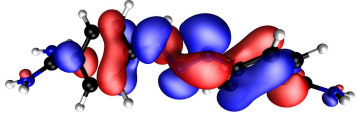

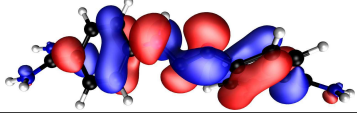

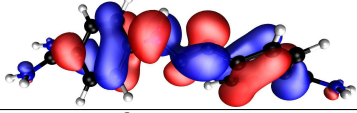
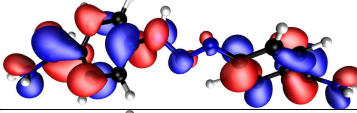
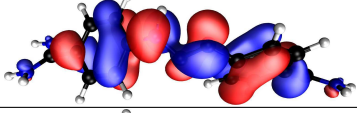

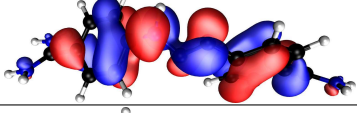
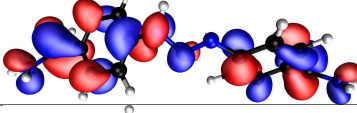
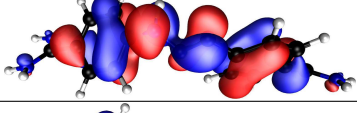
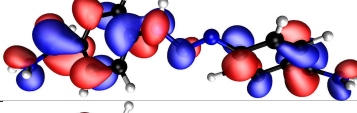
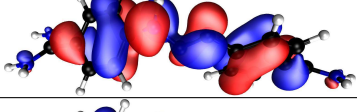
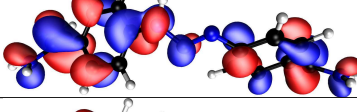
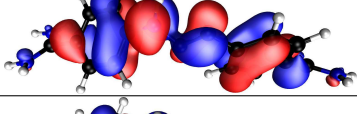
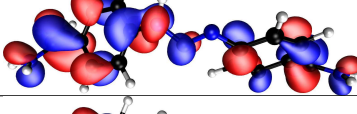
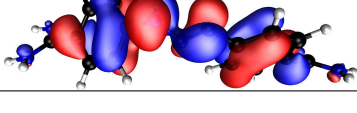
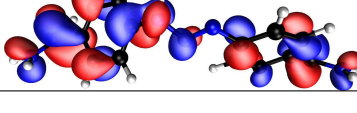
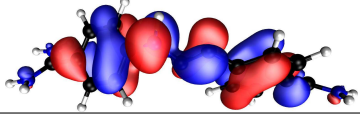
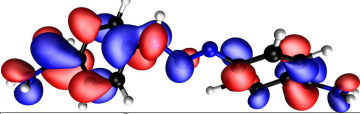
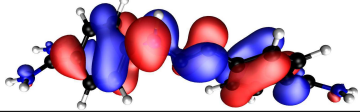
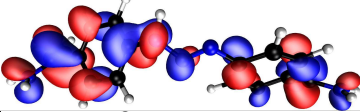
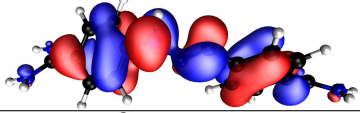
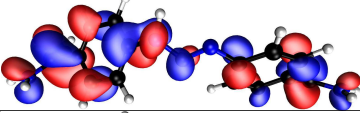
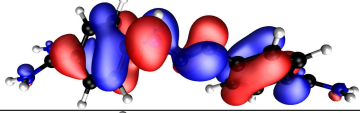
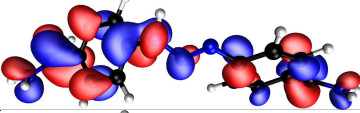
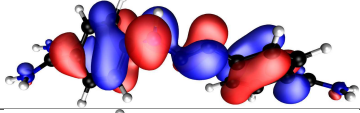
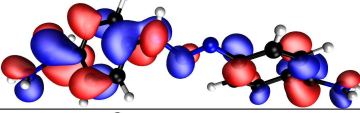
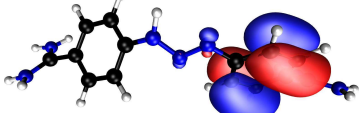
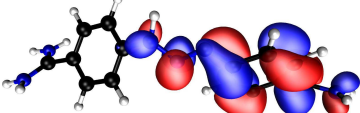
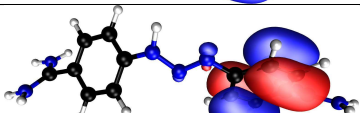
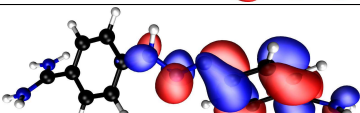
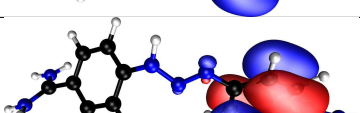
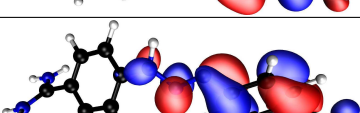
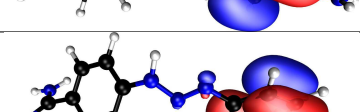
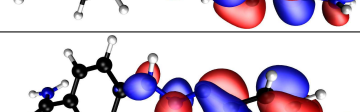
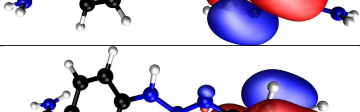
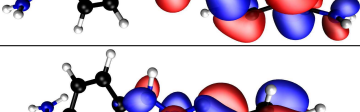
EEL	Step	VEE	OS	OCC	VIR	Contrib.
3	50	3.9	0.06			91.6 %
3	100	4.1	0.06			90.0 %
3	150	4.2	0.07			86.4 %
3	200	4.3	0.07			84.3 %
3	250	4.3	0.08			83.7 %
3	300	4.3	0.08			84.0 %
3	350	4.4	0.09			84.7 %
3	400	4.4	0.09			85.3 %
3	450	4.4	0.09			86.0 %
3	500	4.4	0.09			86.5 %

Table S15: Part II: VEE, OS and NTOs of $S_0 \rightarrow S_3$ excitation for selected IRC₅ steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

EEL	Step	VEE	OS	OCC	VIR	Contrib.
3	550	4.4	0.09			86.9 %
3	600	4.4	0.09			87.3 %
3	650	4.4	0.09			87.6 %
3	700	4.4	0.09			87.8 %
3	750	4.4	0.09			88.0 %
3	1000	4.4	0.01			68.5 %
3	1250	4.4	0.01			68.8 %
3	1500	4.4	0.01			69.0 %
3	1750	4.4	0.01			69.2 %
3	2000	4.4	0.01			69.4 %

$\text{ET}_{S_0} \rightarrow \text{ET}_{S_4}$:

Table S16: Part I: VEE, OS and NTOs of $S_0 \rightarrow S_4$ excitation for selected IRC₅ steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

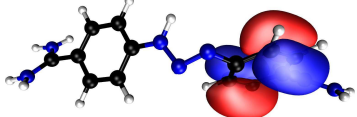
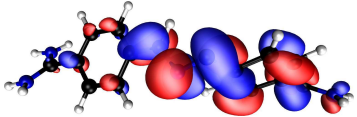
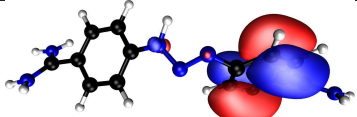
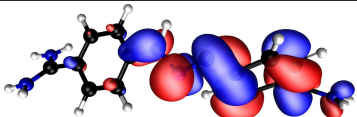
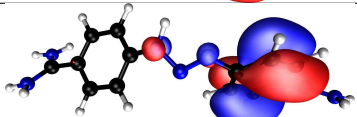
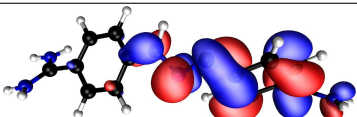
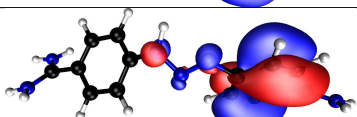
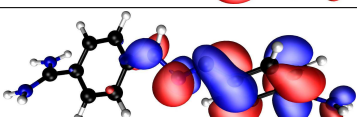
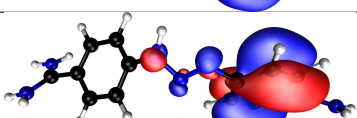
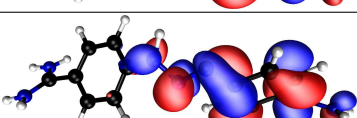
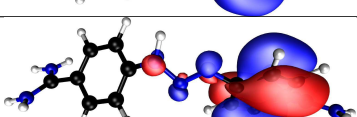
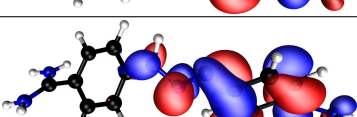
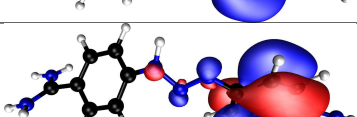
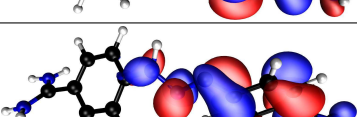
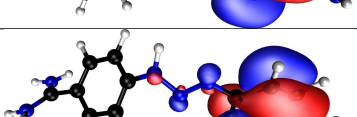
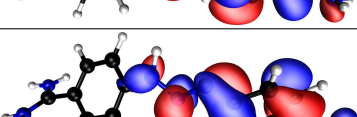

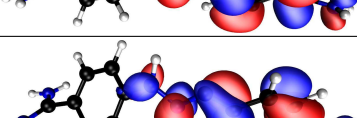
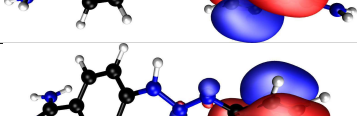
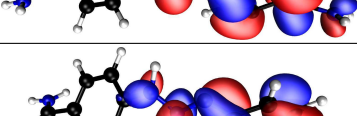

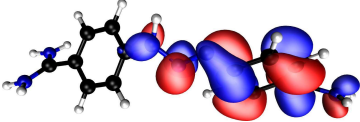
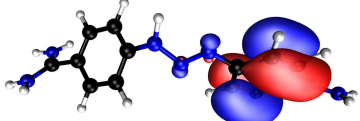
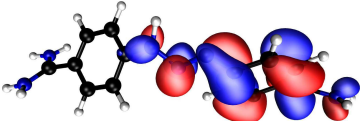
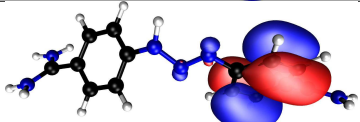
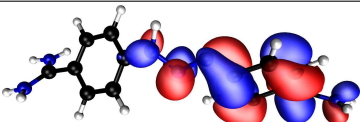
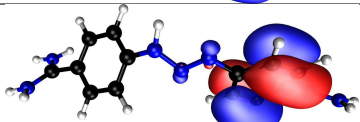
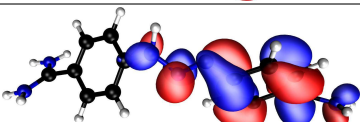
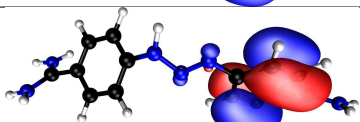
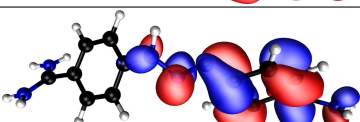
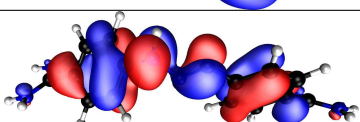
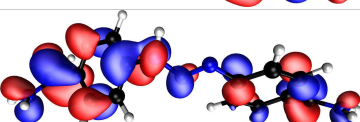
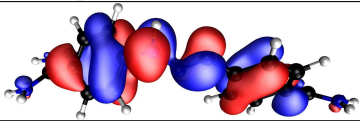
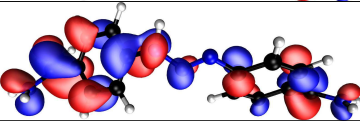
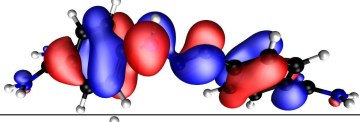
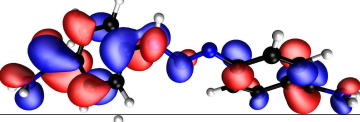
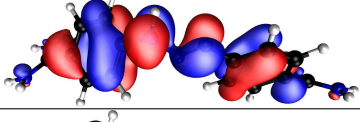
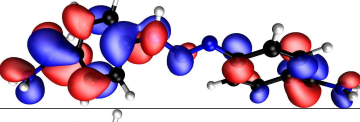
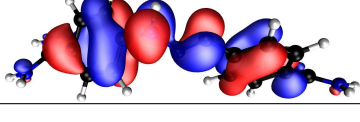
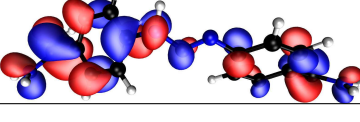
EEL	Step	VEE	OS	OCC	VIR	Contrib.
4	50	4.0	0.01			65.8 %
4	100	4.2	0.02			62.8 %
4	150	4.3	0.02			61.6 %
4	200	4.4	0.02			61.9 %
4	250	4.4	0.01			62.8 %
4	300	4.4	0.01			63.7 %
4	350	4.4	0.01			64.6 %
4	400	4.4	0.01			65.4 %
4	450	4.4	0.01			66.0 %
4	500	4.4	0.01			66.5 %

Table S17: Part II: VEE, OS and NTOs of $S_0 \rightarrow S_4$ excitation for selected IRC₅ steps, calculated at ADC(2)/aTZ level. The isosurfaces chosen to visualize orbitals are at +0.03 (red) and -0.03 (blue). The contribution of each pair is shown in the last column.

EEL	Step	VEE	OS	OCC	VIR	Contrib.
4	550	4.4	0.01			67.0 %
4	600	4.4	0.01			67.3 %
4	650	4.4	0.01			67.5 %
4	700	4.4	0.01			67.7 %
4	750	4.4	0.01			67.9 %
4	1000	4.4	0.08			88.4 %
4	1250	4.4	0.08			88.7 %
4	1500	4.5	0.08			88.9 %
4	1750	4.5	0.08			88.9 %
4	2000	4.5	0.08			89.0 %

Cartesian coordinates

Using the density functional theory (DFT) with the B3-LYP exchange-correlation functional, the D3(BJ) dispersion correction and the def2-TZVP basis set (doubly polarized at C/N/O, singly polarized at H), we could characterize six local minima on the electronic ground state potential energy surface. In the following, the cartesian coordinates of the fully optimized structure of the conformers are given in Ångstrom:

ET1:

```
C 0.6373202 -1.4733267 1.9216467
C 0.6027056 -2.3217136 3.0327754
C 1.7750259 -2.7257418 3.6419229
C 3.0088642 -2.2944832 3.1402925
C 3.0427946 -1.4481924 2.0206057
C 1.8714843 -1.0360610 1.4191671
C 4.2522059 -2.7263590 3.7787217
N 4.2942994 -2.8991091 5.0896963
N 5.3313944 -2.9435784 3.0437789
H 6.2291462 -3.1632454 3.4493684
H 5.0994700 -3.2830552 5.5619762
H 3.5234437 -2.5978582 5.6637233
H 3.9870683 -1.0725591 1.6476528
H 1.9021098 -0.3709042 0.5692244
H -0.3569083 -2.6612411 3.3968240
H 1.7274251 -3.4137899 4.4758304
N -0.6201206 -1.1331461 1.3970827
N -0.6073949 -0.3569461 0.4127433
N -1.8350639 -0.0913909 -0.0218643
H -2.5999920 -0.5379063 0.4805425
```

C -2.0915548 0.7374805 -1.0940043
C -3.4296115 0.9474411 -1.4579467
C -3.7373825 1.7625644 -2.5246511
C -2.7205861 2.4004088 -3.2502455
C -1.3848287 2.1882229 -2.8752047
C -1.0666032 1.3647484 -1.8165517
H -0.0360000 1.1919969 -1.5485320
H -0.5796823 2.6329917 -3.4455798
H -4.7783372 1.9402302 -2.7608219
H -4.2248287 0.4784240 -0.8930008
C -3.0484483 3.2674383 -4.3751678
N -2.2899505 4.3198188 -4.6462592
H -2.4257735 4.8873171 -5.4694781
N -4.1059809 3.0061460 -5.1292033
H -4.4262018 3.6355147 -5.8501036
H -1.5915228 4.6232143 -3.9878855
H 5.2622744 -2.9616326 2.0393634
H -4.5902596 2.1282818 -5.0364385

ET2:

C 0.0156349 0.0590059 0.0467456
C -0.3296413 -0.8138286 1.0832955
C 0.6336506 -1.2768746 1.9586160
C 1.9682380 -0.8838106 1.8022447
C 2.3154204 -0.0152553 0.7553012
C 1.3511181 0.4568623 -0.1112029
C 2.9920767 -1.3799237 2.7218063

N 2.6924243 -1.5823041 3.9944274
N 4.2149450 -1.6253843 2.2788159
H 4.9715577 -1.8900707 2.8921185
H 3.3368195 -2.0093440 4.6434299
H 1.8114700 -1.2620790 4.3629931
H 3.3359114 0.3290085 0.6463710
H 1.6204936 1.1365239 -0.9057595
H -1.3607162 -1.1244304 1.1786264
H 0.3517580 -1.9812422 2.7303250
N -1.0527612 0.4585437 -0.7723406
N -0.7732476 1.2969685 -1.6613848
N -1.8363497 1.6110041 -2.3948519
H -2.7080266 1.1438496 -2.1523555
C -1.7960036 2.5251813 -3.4268538
C -2.9797998 2.7656314 -4.1394577
C -2.9930360 3.6755733 -5.1733209
C -1.8239145 4.3616555 -5.5332848
C -0.6426034 4.1093714 -4.8184930
C -0.6226314 3.2096389 -3.7743892
H 0.2846011 3.0398072 -3.2159140
H 0.2621120 4.6577764 -5.0469304
H -3.9086966 3.8145175 -5.7329367
H -3.8838470 2.2272484 -3.8857915
C -1.8385244 5.3205012 -6.6309850
H -3.6860508 6.0441176 -6.2124212
N -2.9271423 6.0353792 -6.8740023
H -3.0140346 6.6321427 -7.6831087

N -0.7631757 5.4796973 -7.3890239

H -0.6998788 6.1983424 -8.0945362

H 4.4036646 -1.6194491 1.2897236

H 0.0027453 4.8297879 -7.3235758

EC1:

C 0.0877418 -0.3545286 -0.1661107

C 0.3181191 -1.4202164 -1.0399285

C 1.6068861 -1.8437210 -1.3057055

C 2.6942091 -1.1949044 -0.7086211

C 2.4617573 -0.1184350 0.1614514

C 1.1751351 0.2961143 0.4346030

C 4.0610908 -1.6325760 -0.9889628

N 4.3148704 -2.9153217 -1.1933469

N 5.0415257 -0.7452677 -1.0377158

H 6.0101693 -1.0110724 -1.1363701

H 5.2240910 -3.2508407 -1.4750440

H 3.6055204 -3.6056911 -1.0083123

H 3.2879004 0.3680945 0.6640942

H 1.0010587 1.1144897 1.1168015

H -0.5264001 -1.9037692 -1.5105383

H 1.7643078 -2.6465051 -2.0142193

N -1.2663483 -0.0073248 0.0363690

N -1.4214873 0.8888903 0.8993345

N -2.6647077 1.2884167 1.1519468

H -2.6622645 2.0011349 1.8660182

C -3.9123245 0.9282222 0.6487282

C -5.0080270 1.6147692 1.2026122
C -6.2907795 1.3421609 0.7894079
C -6.5227337 0.3787728 -0.2043502
C -5.4305254 -0.2986660 -0.7571977
C -4.1370355 -0.0404805 -0.3399962
H -3.3091081 -0.5820119 -0.7595746
H -5.5862199 -1.0770172 -1.4930839
H -7.1081012 1.9152902 1.2069938
H -4.8428469 2.3755652 1.9553100
C -7.8830735 0.0884884 -0.6489476
N -8.1107615 -0.2459383 -1.9098762
H -9.0192417 -0.5392473 -2.2372279
N -8.8887376 0.1608375 0.2090187
H -9.8522162 0.0609736 -0.0745077
H -7.3834692 -0.1443645 -2.5986601
H 4.8323808 0.2397684 -1.0270033
H -8.7074645 0.2601411 1.1946713

EC2:

C -0.0406970 0.1636545 0.3362151
C -0.2727114 0.2750716 1.7095705
C 0.7741484 0.5115795 2.5809205
C 2.0790500 0.6378783 2.0897812
C 2.3099272 0.5303415 0.7097174
C 1.2635882 0.3024465 -0.1595572
C 3.1934874 0.8806728 3.0054603
N 3.0111559 1.6225658 4.0861681

N 4.3815806 0.3565798 2.7514477
H 5.1986458 0.5683487 3.3048583
H 3.7256766 1.7435616 4.7886566
H 2.1565845 2.1422187 4.2029632
H 3.3046630 0.6748795 0.3078491
H 1.4432518 0.2421724 -1.2223382
H -1.2806693 0.1568562 2.0818940
H 0.5788102 0.5491478 3.6446960
N -1.1805292 -0.0731903 -0.4636291
N -0.8987919 -0.3192847 -1.6603234
N -1.9095987 -0.5468906 -2.4944154
H -1.5586817 -0.7490109 -3.4184749
C -3.2938844 -0.5743093 -2.3439239
C -4.0212295 -0.8946340 -3.5045006
C -5.3946433 -0.9556192 -3.4794049
C -6.0915957 -0.6842102 -2.2920301
C -5.3658894 -0.3589752 -1.1409614
C -3.9834508 -0.3079947 -1.1522364
H -3.4375217 -0.0764901 -0.2560202
H -5.8779972 -0.1871390 -0.2029783
H -5.9262899 -1.1676943 -4.3977091
H -3.4978253 -1.0862004 -4.4329171
C -7.5503235 -0.7441971 -2.2617741
H -7.6814153 -2.3555286 -3.4840318
N -8.1912565 -1.6258031 -3.0131167
H -9.1970039 -1.6385305 -3.0967723
N -8.2312436 0.0832940 -1.4838155

H -9.2312169 0.0162129 -1.3648512
H 4.4867690 -0.3221849 2.0148937
H -7.7651523 0.8572249 -1.0393801

ZT1:

C 5.0879085 -0.6002451 -0.8172036
C 4.6790946 -1.9338557 -0.6776537
C 5.4924090 -2.9658400 -1.1613842
C 6.6961312 -2.6731857 -1.7689090
C 7.1119582 -1.3432704 -1.9182377
C 6.2870327 -0.3167535 -1.4342656
N 3.4745738 -2.2585293 -0.0699187
N 2.7036725 -1.2818068 0.4473822
N 1.6408595 -1.5587020 1.0202454
C 1.0900607 -2.8551908 1.1295479
C 0.4292378 -3.4432393 0.0431095
C -0.3102602 -4.5963054 0.2286863
C -0.3899140 -5.1917406 1.4948493
C 0.2952870 -4.6124454 2.5720018
C 1.0189048 -3.4491747 2.3946531
C -1.2150426 -6.3824692 1.7021504
N -0.8454431 -7.3002386 2.5808098
C 8.3805969 -1.0284305 -2.5660173
N 9.4120521 -1.8506906 -2.4419262
N -2.3335986 -6.5357284 1.0121601
N 8.5028471 0.0803789 -3.2794967
H -1.4345626 -8.0808342 2.8310369

H -2.8952263 -7.3727503 1.0684010
H -2.7018022 -5.7714500 0.4690197
H 0.2097984 -5.0285284 3.5675661
H 1.4959782 -2.9654615 3.2359589
H 0.4689990 -2.9731330 -0.9304948
H -0.8031367 -5.0470115 -0.6231829
H 3.2124735 -3.2326219 0.0460349
H 4.4687668 0.1942300 -0.4306906
H 6.6036148 0.7163827 -1.4961976
H 7.2894222 -3.4846929 -2.1695650
H 5.1757337 -3.9970520 -1.0707521
H 9.3867629 0.3871707 -3.6577165
H 10.2750042 -1.7170640 -2.9477540
H 7.6895045 0.6282678 -3.5080428
H 0.0654455 -7.2560313 3.0074756
H 9.3830862 -2.6011970 -1.7716398

ZT2:

C -2.7226046 -4.1060622 1.4363783
C -3.3327211 -3.8123297 0.2089533
C -4.5747258 -4.3777380 -0.1043226
C -5.1982642 -5.2215718 0.7916870
C -4.5919404 -5.5307732 2.0166590
C -3.3465209 -4.9602113 2.3196301
N -2.7311394 -2.9639145 -0.7096074
N -1.4987852 -2.4781987 -0.4614496
N -0.9344260 -1.7485909 -1.2881279

C -1.5079365 -1.2965274 -2.4977398
C -0.9864509 -1.7713316 -3.7064380
C -1.3720296 -1.1924490 -4.9000025
C -2.2675160 -0.1138744 -4.9074535
C -2.7916225 0.3535905 -3.6946218
C -2.4233035 -0.2359889 -2.4997806
C -2.6165468 0.5442547 -6.1670657
N -2.8272127 1.8503109 -6.1901555
C -5.2409870 -6.4330800 2.9615021
N -4.5091450 -7.2237047 3.7313935
N -2.7159512 -0.1646046 -7.2800005
N -6.5625631 -6.4639750 3.0506059
H -3.1407808 2.3346787 -7.0185709
H -2.8492505 0.2617573 -8.1852412
H -2.6902799 -1.1704995 -7.2445639
H -3.5111340 1.1621909 -3.6815622
H -2.8113796 0.1425596 -1.5635331
H -0.2481090 -2.5612901 -3.6925090
H -0.9192081 -1.5393181 -5.8198950
H -3.1870350 -2.7729186 -1.5965550
H -1.7739283 -3.6568240 1.6855275
H -2.8767409 -5.1455719 3.2768985
H -6.1376677 -5.6791942 0.5103378
H -5.0442798 -4.1675829 -1.0568227
H -7.0512356 -7.1378685 3.6211242
H -4.9100021 -7.7873720 4.4663122
H -7.1170179 -5.7567102 2.5970512

H -2.5934891 2.4146526 -5.3891697

H -3.5211994 -7.3220193 3.5631077

Cartesian coordinates of ground and excited state structures of ET photoisomerization

Photoisomerization processes of ET conformer is discussed in the main text. Geometries are optimized at ADC(2)/cc-pVTZ level. All the cartesian coordinates are given in atomic units.

ET_{S0}:

1.16116089405767 -2.88854397771015 3.58258578997744 c
1.11995781081754 -4.17351617065118 5.89306988609260 c
3.35803510023253 -4.86908476954957 7.06584969494578 c
5.66607071687493 -4.31287908477889 5.89676541894258 c
5.71637197918228 -3.05379318391236 3.56337184197663 c
3.47427316507424 -2.33723640026719 2.41359535070285 c
8.03182760244579 -5.07254155423343 7.10707849007501 c
8.23831150201761 -4.93777985080908 9.58883673409645 n
9.92787207621832 -5.88349464313283 5.70260290850901 n
11.63507324024509 -6.30957926256569 6.43528719352712 h
9.77015710767721 -5.57669556830067 10.52610162655365 h
6.87354065630066 -4.07691498327741 10.59627592456871 h
7.49875152941691 -2.56557174763087 2.68754672592539 h
3.50087125730493 -1.36004273354585 0.62285865937780 h
-0.68740330825702 -4.62346391184551 6.73118283736718 h
3.29932264918981 -5.92221941718435 8.81730202541472 h
-1.23633625596999 -2.30813983540025 2.58875638488550 n
-1.17302998563904 -0.78231586985728 0.72836247665453 n
-3.48758775588157 -0.36691991897404 -0.15179779541686 n
-4.92257356990123 -1.29903047162357 0.72805384242068 h

-3.96090895222203 1.28123008842525 -2.11858586804722 c
-6.46657089569302 1.56714168033406 -2.92794022948380 c
-7.03968617813244 3.18473077413830 -4.90168253027906 c
-5.11132264414079 4.56168693567207 -6.08207301313388 c
-2.60723763591727 4.28501923922600 -5.26190164081466 c
-2.02633649609264 2.65032947584062 -3.30199828664837 c
-0.09588130983678 2.41656442221215 -2.69074664548345 h
-1.08934308135921 5.27487148929407 -6.20911960287088 h
-8.99345629318345 3.43813383367752 -5.44758040231869 h
-7.96729834219376 0.53636847528224 -1.99714596379543 h
-5.71305868020993 6.27880480729839 -8.15261279633656 c
-4.44545626214488 8.41667281544795 -8.39344509218261 n
-4.69189967303102 9.58872238551303 -9.87567415681420 h
-7.52055885485326 5.68052257823862 -9.76706127683638 n
-8.11465971750557 6.87715489738054 -11.12609952226576 h
-3.29404688082464 8.98540653722798 -6.99131592691866 h
9.63933914864983 -6.23503233492734 3.85592478288492 h
-8.26628385168840 3.93143449907823 -9.73462822319729 h

ET_{TSS1}:

1.41004088206089 -2.63971576335239 3.49394468659848 c
1.27207336422814 -4.31849237666641 5.64630372804097 c
3.41471529249501 -5.13764270235405 6.83782444632073 c
5.82496627625781 -4.37052889817445 5.96206355809147 c
6.01268257133904 -2.73755107538374 3.85306874784070 c
3.89036149053884 -1.87374266238384 2.64550870550017 c
8.08714595265297 -5.24812370195873 7.22835171275797 c

8.02890985412436 -5.76439896410564 9.67834690972025 n
10.21670539995263 -5.53689100214506 5.93984280293854 n
11.86354532921572 -5.97896839955850 6.78892760963036 h
9.50869385595337 -6.54813196837528 10.58655295856362 h
6.52885437473846 -5.23707107966001 10.71990182975088 h
7.84599357324963 -2.06755528175638 3.23878668182634 h
4.03067531000175 -0.58885807855293 1.06778755702735 h
-0.57944540544499 -4.92416178070158 6.26191301621532 h
3.25110570607324 -6.46325792884470 8.38698679234684 h
-0.73566853616308 -1.95961541256840 2.50134425334673 n
-0.29105368044483 -0.15098577454298 0.18487132510321 n
-2.67170778352526 0.21589375672489 -0.40536908388131 n
-3.94778488518872 -0.70674948283981 0.73198124882570 h
-3.43744531221933 1.71334073219361 -2.38865569069795 c
-6.04119489875116 1.98053343796420 -2.83644788630606 c
-6.86744809704484 3.46408417171432 -4.82208836527693 c
-5.10266691908308 4.71193010880272 -6.36286912932854 c
-2.50267016683027 4.44573051250984 -5.89903153621753 c
-1.65934665208562 2.94598480164557 -3.93055670571255 c
0.33506298116954 2.69286496819060 -3.57806998882330 h
-1.13332887082334 5.33358002571112 -7.13121926163043 h
-8.87483504762006 3.72408204567386 -5.10968777188981 h
-7.39480807462147 1.04738142139944 -1.61940965484455 h
-5.97631783216945 6.28767339352160 -8.45462168619502 c
-4.73556432443422 8.37773342631446 -9.02643994234491 n
-5.18153891632162 9.44740990108928 -10.54033471559842 h
-7.99823616702308 5.60554765817384 -9.75051848731763 n

-8.75912775146470 6.70536203598136 -11.10943284680919 h
-3.39403938484978 9.02911294279231 -7.84591799585762 h
10.18413532916597 -5.48881712495609 4.04044553486010 h
-8.74387905303352 3.87478874580283 -9.49189512115557 h

ET_{S1}:

1.41004088206089 -2.63971576335239 3.49394468659848 c
1.27207336422814 -4.31849237666641 5.64630372804097 c
3.41471529249501 -5.13764270235405 6.83782444632073 c
5.82496627625781 -4.37052889817445 5.96206355809147 c
6.01268257133904 -2.73755107538374 3.85306874784070 c
3.89036149053884 -1.87374266238384 2.64550870550017 c
8.08714595265297 -5.24812370195873 7.22835171275797 c
8.02890985412436 -5.76439896410564 9.67834690972025 n
10.21670539995263 -5.53689100214506 5.93984280293854 n
11.86354532921572 -5.97896839955850 6.78892760963036 h
9.50869385595337 -6.54813196837528 10.58655295856362 h
6.52885437473846 -5.23707107966001 10.71990182975088 h
7.84599357324963 -2.06755528175638 3.23878668182634 h
4.03067531000175 -0.58885807855293 1.06778755702735 h
-0.57944540544499 -4.92416178070158 6.26191301621532 h
3.25110570607324 -6.46325792884470 8.38698679234684 h
-0.73566853616308 -1.95961541256840 2.50134425334673 n
-0.29105368044483 -0.15098577454298 0.18487132510321 n
-2.67170778352526 0.21589375672489 -0.40536908388131 n
-3.94778488518872 -0.70674948283981 0.73198124882570 h
-3.43744531221933 1.71334073219361 -2.38865569069795 c

-6.04119489875116 1.98053343796420 -2.83644788630606 c
-6.86744809704484 3.46408417171432 -4.82208836527693 c
-5.10266691908308 4.71193010880272 -6.36286912932854 c
-2.50267016683027 4.44573051250984 -5.89903153621753 c
-1.65934665208562 2.94598480164557 -3.93055670571255 c
0.33506298116954 2.69286496819060 -3.57806998882330 h
-1.13332887082334 5.33358002571112 -7.13121926163043 h
-8.87483504762006 3.72408204567386 -5.10968777188981 h
-7.39480807462147 1.04738142139944 -1.61940965484455 h
-5.97631783216945 6.28767339352160 -8.45462168619502 c
-4.73556432443422 8.37773342631446 -9.02643994234491 n
-5.18153891632162 9.44740990108928 -10.54033471559842 h
-7.99823616702308 5.60554765817384 -9.75051848731763 n
-8.75912775146470 6.70536203598136 -11.10943284680919 h
-3.39403938484978 9.02911294279231 -7.84591799585762 h
10.18413532916597 -5.48881712495609 4.04044553486010 h
-8.74387905303352 3.87478874580283 -9.49189512115557 h

ET_{TSS0}:

0.30913207700871 -4.39203283389735 -0.59358161831200 c
-1.82713629762837 -5.85058156929214 0.09859755944527 c
-1.60018168053120 -8.42738406581227 0.40579099295239 c
0.72439098309633 -9.65105903411675 0.01778571322016 c
2.84037625579005 -8.20185225144759 -0.66964335448205 c
2.66175667245262 -5.61871628240561 -0.95790073686041 c
0.92924228076117 -12.36254858207543 0.29865538167812 c
-0.53094258310090 -13.57250478163112 1.93489242577846 n

2.57723603878503 -13.64712186327509 -1.08216846098374 n
2.91075348228555 -15.50051632520921 -0.80158548606385 h
-0.59485306177165 -15.47305296641557 2.02760422595388 h
-1.53305841562309 -12.58428228848118 3.21073932564162 h
4.67486615418054 -9.07929292007752 -0.88895326930256 h
4.30659871787652 -4.51876878012040 -1.45964769648396 h
-3.63757587830136 -4.93713582267369 0.33242099714890 h
-3.28357614287312 -9.50499844415354 0.83939112039229 h
0.08543378930061 -1.92775127509908 -0.99011935070120 n
-0.04591251004878 0.36153794280077 -1.33833612798924 n
0.45613055077561 1.83349183473002 0.69659811335520 n
0.90904573252207 0.98447134584442 2.35983297271007 h
0.30605625602423 4.44798446331489 0.49296205968727 c
0.88687700861072 5.91265666187019 2.61663673221834 c
0.74827453337309 8.52523359288757 2.49352337109229 c
0.04991466636710 9.70229833432622 0.22993627184633 c
-0.51954118504141 8.23127997146806 -1.89673398501123 c
-0.40784676366850 5.61840518588529 -1.77212546292795 c
-0.88675011562630 4.49004303332840 -3.40088160896262 h
-1.14627659911390 9.11030177632123 -3.63302339177911 h
1.27759477377879 9.62995104974367 4.13010236477032 h
1.46929073070902 5.01538182870074 4.35908778798072 h
-0.08446142138015 12.45532027373939 0.08467118726034 c
0.60262928270997 13.61218462116686 -2.01649950865123 n
0.40036013733890 15.49145338265911 -2.26219143803140 h
-0.89082217237440 13.75576604492708 2.05597104132533 n
-0.87513392138202 15.66122461582199 2.09941967669269 h

1.47384888423070 12.62536328900001 -3.38915031377314 h
3.42749628017240 -12.80296626913284 -2.55677160247281 h
-1.67577227336428 12.84038647585802 3.52646030618991 h

ZT_{so}:

-4.16368272146639 0.68569582005777 2.48234198048722 c
-5.34641279721484 -0.42673719943778 0.39032066507617 c
-6.68888973777109 -2.66252113116163 0.68342002287593 c
-6.82625393037054 -3.81321694745062 3.06474555909407 c
-5.59970337327184 -2.72770194288235 5.14608028425104 c
-4.29514095298274 -0.47105826924064 4.85684390461212 c
-8.33440750736698 -6.10797658616524 3.40492026253538 c
10.47197915943034 -6.36274209346897 2.14637588611647 n
-7.54570970779231 -7.88249480946906 4.96978981201289 n
-8.59812634811571 -9.41420155504056 5.39520968336343 h
11.52708374620515 -7.94857777644562 2.23248560373151 h
11.18337903434761 -4.87558299586366 1.19627884520339 h
-5.77579618015650 -3.55328133841993 7.00869791781521 h
-3.44674065774659 0.45346321818996 6.46935836318763 h
-5.27134115891459 0.49853677693893 -1.43154937080243 h
-7.57934739987552 -3.52436021379180 -0.94356047821942 h
-3.18844306332789 3.18003982916017 2.33120489691345 n
-1.14605294815310 3.66214316970230 1.19924647112248 n
0.21689199409366 1.76093506083325 0.20141551501055 n
-0.31381680333981 -0.06355885978086 0.47389814967314 h
2.51107318763900 2.31920249035304 -0.94869127364282 c
4.00928982873828 0.33659442830994 -1.85431304310059 c

6.30507974614055 0.83738224701836 -3.01189313169169 c
7.11820527954458 3.33922582325174 -3.29827678076040 c
5.60910343797466 5.32189926981904 -2.40063437989874 c
3.32475165490952 4.82526658093161 -1.22498321824409 c
2.17919835034595 6.34808802319889 -0.50143334915542 h
6.25057172967314 7.25914351117916 -2.52963199901746 h
7.40259299987174 -0.71309004597053 -3.76768664189533 h
3.37481711421112 -1.59889520233580 -1.67231351924238 h
9.52637210780900 3.88652018003571 -4.52676374022747 c
9.74319115847393 5.91486226011123 -5.96387533092943 n
11.40603337033828 6.46128923260021 -6.71802572426053 h
11.46377640897257 2.34815611827066 -4.18935295022813 n
13.11693849872122 2.57017890778772 -5.11114794079420 h
8.18878464464898 6.90992155490405 -6.42308766293347 h
-5.80550550955466 -7.76282941388498 5.72708414271126 h
11.36114122529806 0.99028112226582 -2.86249667485892 h

Cartesian coordinates of ground and excited state structures of EC photoisomerization

Photoisomerization processes of EC conformer is discussed in the main text. Geometries are optimized at ADC(2)/aug-cc-pVDZ level. All the cartesian coordinates are given in atomic units.

EC_{s0}:

-0.46267381236836 -1.91656554916203 1.50725277464401 c
0.18858612398804 -4.06572509692792 0.04155442386153 c
2.39190679391185 -4.06960070842611 -1.42957121398629 c
3.95309068450610 -1.90613697376833 -1.42469836398145 c
3.31602259064578 0.26608074731928 0.00672409507728 c
1.12046591981248 0.25892616939820 1.47791685285659 c
6.33496470200943 -1.92789499398483 -2.88659140280371 c
7.76771126289014 -3.99035948653669 -2.85841802355710 n
7.00264954665786 0.11308984406105 -4.19039460764827 n
8.69010871185995 0.25365961459979 -5.09858809323669 h
9.36435732749795 -4.15471001203305 -3.91513367084487 h
7.35532720937878 -5.41068358234437 -1.63724044324988 h
4.59102804570089 1.89325921892822 0.07389823039056 h
0.65929809192784 1.87768038112515 2.67072884739218 h
-1.04677081385054 -5.72110960945521 0.10754375826107 h
2.85737317335045 -5.71619490007529 -2.59022386172411 h
-2.58055215424160 -2.19772395202736 3.04772190991950 n
-3.01741573265787 -0.11856444380529 4.60382073675501 n
-4.53659863874689 1.65029957406055 3.41596722497882 n
-4.57890791347018 3.25654147380911 4.48628230349042 h

-6.69476556130878 1.20748449599392 1.95555030319601 c
-8.07267250998813 3.37051218022572 1.15003556578181 c
-10.32138313752887 3.09720178562578 -0.19669941612561 c
-11.22365968817472 0.64894404283441 -0.81214154750931 c
-9.82564287050574 -1.50335545999226 -0.05457552604360 c
-7.57902725699563 -1.24298147407734 1.31721587073350 c
-6.57213622711267 -2.91471242861191 1.98862078191481 h
-10.55513055654332 -3.40616912110493 -0.40936244675364 h
-11.32484554101993 4.78826827320462 -0.83723640485586 h
-7.36955578724291 5.26256520437090 1.60131771218942 h
-13.62800904834184 0.34869820609368 -2.15628417249781 c
-13.91422257297715 -1.52064119448963 -3.82333416000648 n
-15.60347907280847 -1.91611551859286 -4.64538719065035 h
-15.52337837185873 1.94439036587313 -1.69603483533113 n
-17.16566998753476 1.90549427865933 -2.69006578924774 h
-12.38562262163986 -2.52659964616782 -4.38835468013303 h
5.76456095271614 1.56498785298158 -4.37366056716739 h
-15.41436395870891 3.13716404952678 -0.19994834617066 h

EC_{S1}:

3.11181166236773 -1.57783947185685 1.94863194312843 c
3.75792545163146 -3.72161985127939 0.47295972264576 c
5.95931281170625 -3.72248230028726 -1.00119352100815 c
7.52323301662063 -1.56103919856183 -0.98979459639572 c
6.89109803638572 0.60619048655640 0.45154643428678 c
4.69764357726323 0.59570051760274 1.92602267588197 c
9.90294257406697 -1.57983630267204 -2.45533197516888 c

11.33556126534984 -3.64239397141813 -2.43330420896535 n
10.56844111688951 0.46376556512431 -3.75610395277412 n
12.25451880319038 0.60655807147435 -4.66652408857342 h
12.93078463963630 -3.80495361768572 -3.49245559505642 h
10.92248240921438 -5.06660324638093 -1.21689283610024 h
8.16829103884128 2.23145760696676 0.52331391837819 h
4.23993108986025 2.21025758797841 3.12588181988776 h
2.52039314904011 -5.37557995675929 0.53355067783877 h
6.42138854986557 -5.36518591532850 -2.16869945045265 h
0.99588635808648 -1.86310016076640 3.49143747303764 n
0.56552451455807 0.20758975815522 5.06006462564199 n
-0.95162757136755 1.98695626580638 3.88616721602768 n
-0.98921134568519 3.58674843989244 4.96613851971392 h
-3.10372442766963 1.56268780969925 2.41309369231778 c
-4.47504202094358 3.73616508451999 1.62371028504084 c
-6.71946440682278 3.48024031198175 0.26660553045876 c
-7.62454224624506 1.03982155872622 -0.37583309388560 c
-6.23285576105378 -1.12237735556305 0.36537460505526 c
-3.99049832193206 -0.87981198965262 1.74710217041203 c
-2.98903671597925 -2.55992486521609 2.40571096937117 h
-6.96480423965671 -3.02031648560767 -0.00992997298742 h
-7.71756739282568 5.17952034570584 -0.36046429274800 h
-3.77028488455065 5.62245883441141 2.09607857930545 h
-10.02506804483823 0.75725662481367 -1.73037319683158 c
-10.30915229625338 -1.09442126883168 -3.41748238308204 n
-11.99670654557625 -1.47960342483557 -4.24783763714938 h
-11.91954214240223 2.35092716583434 -1.25943947755853 n

-13.55827863830889 2.32602080821307 -2.25973185304468 h
-8.78104999872463 -2.09962259007519 -3.98510170227387 h
9.33135945716416 1.91755955954169 -3.93095233961074 h
-11.81142898196843 3.53114228386809 0.24661261612168 h

EC_{RS1}:

3.23362486102399 0.78329801015139 -2.21651335957939 c
4.34885416555142 -1.60601392273275 -2.70395050776994 c
6.57389555386669 -2.32870301643782 -1.45937480704135 c
7.70673728806532 -0.62516684111901 0.25288827802523 c
6.60747588905391 1.76130267450601 0.77379284253641 c
4.37470020435485 2.46380577479970 -0.45195111634066 c
10.12529613054172 -1.31376960228738 1.47209789505085 c
10.45270113478600 -3.64978719983334 2.33661681073226 n
11.93216314486934 0.41955171993789 1.66683027076394 n
13.58881418810168 0.08823689593753 2.58264970895222 h
12.12970337842492 -4.26428498895082 3.04519286008632 h
8.96536449409991 -4.85795799265496 2.38327117525829 h
7.46722369768329 3.03673267869390 2.15652474104451 h
3.52560446215410 4.30996835864323 -0.09626839183588 h
3.47507236171535 -2.83696371857116 -4.11540481109830 h
7.47549814729430 -4.13063912629139 -1.92318433785422 h
1.13525170788739 1.37477850059518 -3.69476326421430 n
0.25981659033850 3.82921109854333 -3.32848757185773 n
-1.50760737516373 3.94283749851911 -1.40372928940560 n
-1.89483242002645 5.79529622390524 -1.02321966268465 h
-3.45130229196828 2.24331949072299 -0.85685121983750 c

-5.20474644337125 2.98970548293195 1.04080721226324 c
-7.27053926689685 1.46314295966173 1.62875693542617 c
-7.63074697226303 -0.85833977782270 0.33683187862387 c
-5.86625908196998 -1.61942470631668 -1.52508793280256 c
-3.78191560218528 -0.10314183632072 -2.11571578596032 c
-2.45108221713251 -0.68962818834546 -3.58047054437711 h
-6.08233666874218 -3.43235586350499 -2.49709725830725 h
-8.65406175925918 2.13307822499236 3.01207199824417 h
-4.96727667597552 4.80643980602173 2.00096030029245 h
-9.85046335118128 -2.42404631827281 0.88366492208479 c
-10.98366149511405 -3.68132800167518 -0.98429505577050 n
-12.43353957060381 -4.90060047905340 -0.67156145845283 h
-10.73234282328177 -2.57783619574328 3.24005747301397 n
-12.37769193151619 -3.47014129854416 3.66758072122550 h
-10.52553195386226 -3.28681389025417 -2.80286847026388 h
11.73663281786230 2.09492308768829 0.75365812288900 h
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TS₅₀:

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5.90211857985114 -4.25546913012350 5.98923420095768 c
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3.48396994848504 -1.82821365988494 2.94316524790640 c
8.33792436337775 -4.82152109459849 7.21881132730182 c
8.42520879982951 -5.02842777934446 9.70557477420710 n

10.38050818673814 -5.10552529926850 5.80980145538851 n
12.13031649222402 -5.37176712483172 6.55944068795078 h
10.02365454142249 -5.52447484099510 10.65123180568386 h
6.88349785669153 -4.57214581172942 10.75173573961838 h
7.49037607764545 -1.36956298986623 3.51856884841636 h
3.35159464474755 -0.36662382211273 1.49513636218490 h
-0.35441304153336 -5.85818300959647 6.23730650287699 h
3.79258209739559 -6.99241594684461 8.23053623967551 h
-1.18155708324502 -2.56038934068084 2.80690609275793 n
-1.18431532007569 -1.41507398321075 0.73783807995728 n
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-7.03710872516690 -4.58168900829116 -6.08807271675332 c
-5.08881804784764 -5.75538583286015 -4.70739039508986 c
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-9.25788158862152 -1.13784252186380 -6.53580118706038 h
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4.17837946680116 2.49300984489868 3.84016137096536 h
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4.34700932377045 -4.72658466703074 -2.30138722643857 h
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