Electronic Supplementary Material (ESI) for Faraday Discussions.

Supporting Information

(Total of 16 pages)

for

Photoinduced Formation Mechanism of the Thymine-Thymine (6-4) Adduct in DNA; a QM(CASPT2//CASSCF):MM(AMBER) study

Angelo Giussani,[a,*] Irene Conti,[a,b] Artur Nenov,[a,b] Marco Garavelli[a,b,*]
[a] Dipartimento di Chimica "G. Ciamician", Università di Bologna, Via F. Selmi 2, 40126 Bologna, Italy
[b] Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Viale del Risorgimento , 40136 Bologna, Italy

*To whom correspondence should be addressed. Email: angelo.giussani@uv.es

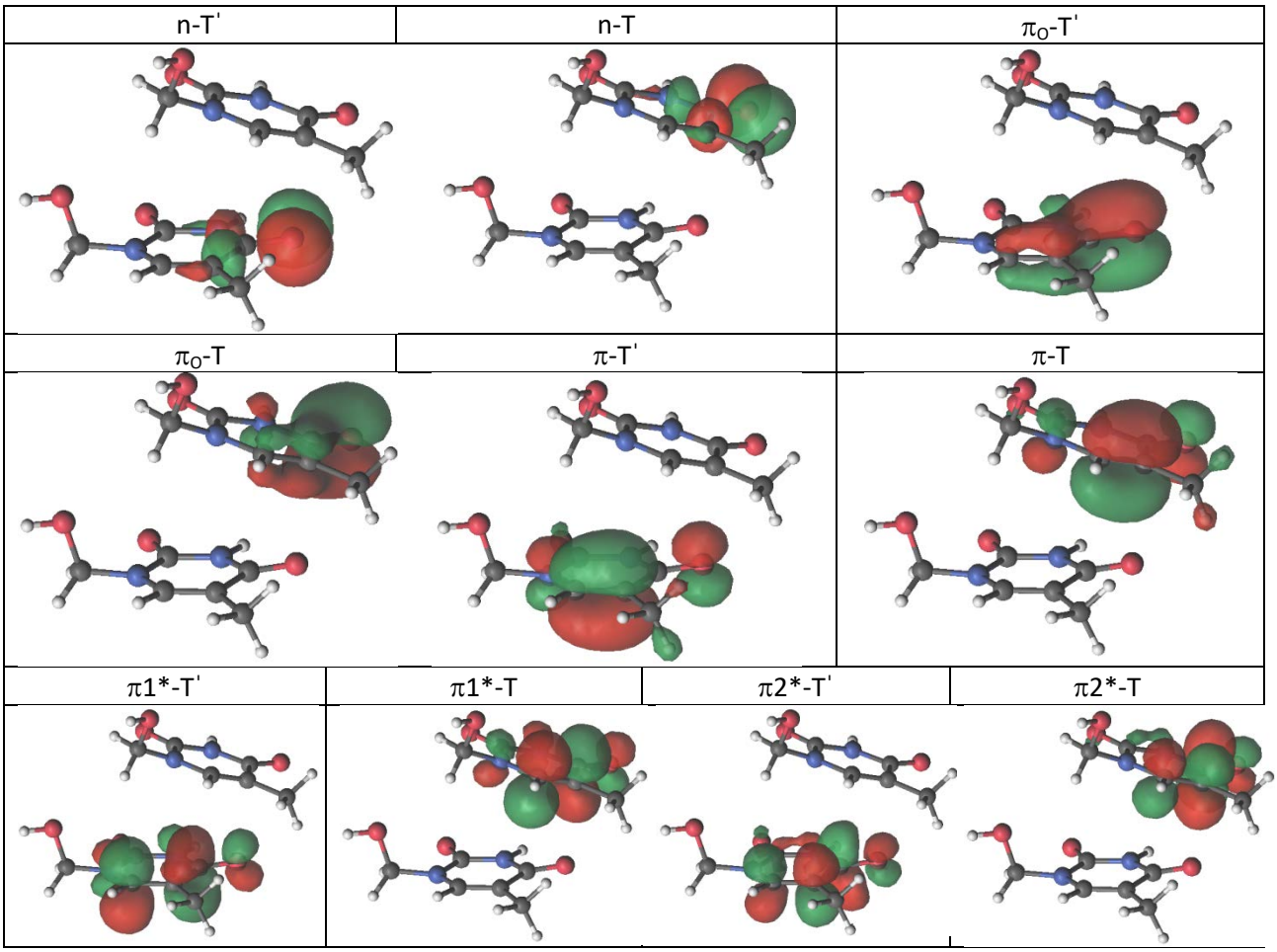


Figure S1. Orbitals forming the active space in the vertical CASPT2(12,10)/Amber computations, characterizing the obtained critical points. Orbitals n-T', n-T, π-T', π-T, π1*-T', π1*-T constitute the CASSCF(8,6) active space employed in the CASSCF(8,6)/Amber optimizations.

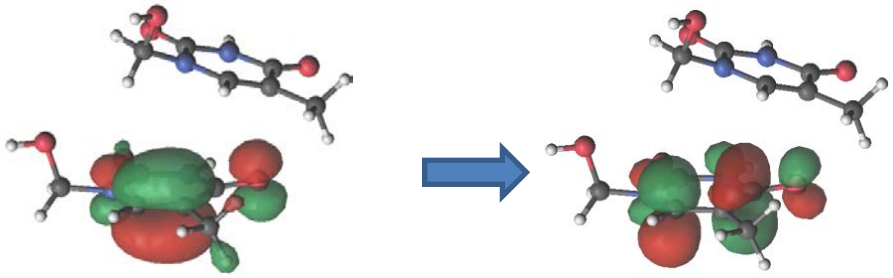


Figure S2. Orbitals mainly describing the $^1\pi\pi^*$-T' and $^3\pi\pi^*$-T' states. The analogous orbitals localized on the T thymine describes the state $^1\pi\pi^*$-T and $^3\pi\pi^*$-T states.

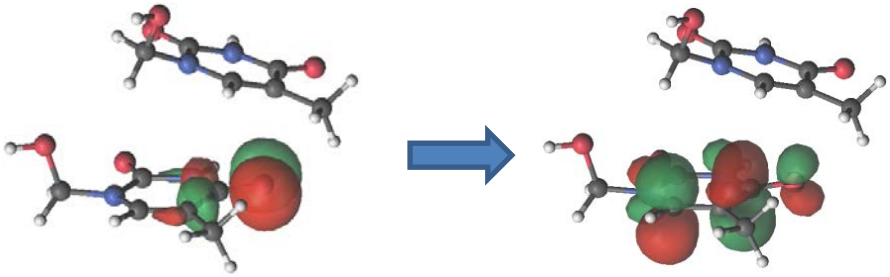


Figure S3. Orbitals mainly describing the $^1n\pi^*$-T' and $^3n\pi^*$-T' states. The analogous orbitals localized on the T thymine describes the state $^1n\pi^*$-T and $^3n\pi^*$-T states.

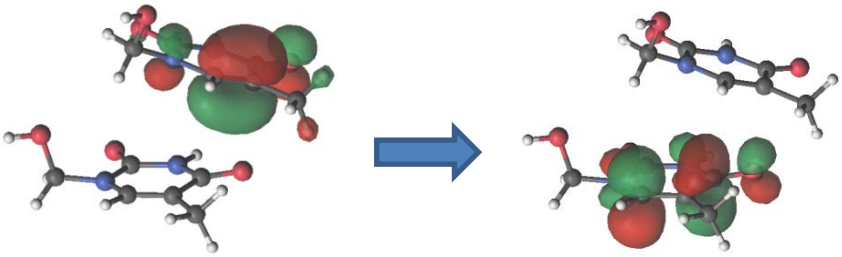


Figure S4. Orbitals mainly describing the ct-$\pi\pi^*$-TT' state.

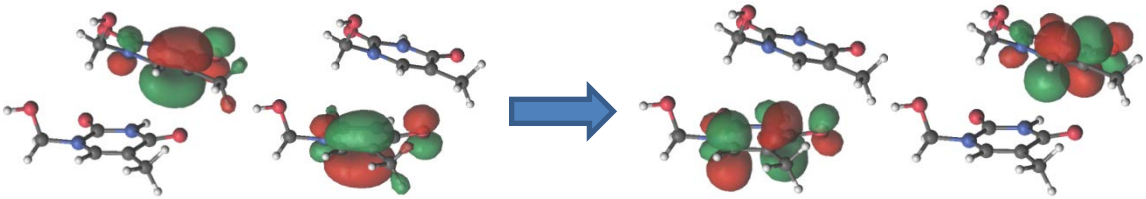


Figure S5. Orbitals mainly describing the double-excited $2\pi2\pi^*$ state.

Table S1. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $^1(gs)_{min}$ (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States.

$^1(gs)_{min}$ geometry			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0 (gs)	0.00	T1 ($^3\pi\pi^*$-T')	3.93
S1 ($^1\pi\pi^*$-T')	4.90	T2 ($^3\pi\pi^*$-T)	3.97
S2 ($^1\pi\pi^*$-T)	5.21	T3 ($^3n\pi^*$-T)	5.21
S3 ($^1n\pi^*$-T)	5.25	T4 ($^3n\pi^*$-T')	5.23
S4 ($^1n\pi^*$-T')	5.27	T5 ($^3\pi_O\pi^*$-T')	6.18
S5 (d)	6.24	T6 ($^3\pi_O\pi^*$-T)	6.30
S6 (ct-$\pi\pi^*$-TT')	7.05	T7	7.76
S7 ($^1\pi_O\pi^*$-T')	7.17	T8	8.28
S8 (np)	7.59	T9	8.33
S9 ($^1\pi_O\pi^*$-T)	7.99	T10	8.99

Table S2. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $^1n\pi^*$-T' state minimum (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

$^1n\pi^*$-T' state minimum			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0 (gs)	1.59	T1 ($^3\pi\pi^*$-T')	4.25
S1 ($^1n\pi^*$-T')	4.80	T2 ($^3n\pi^*$-T')	4.71
S2 ($^1\pi\pi^*$-T')	5.87	T3 ($^3\pi\pi^*$-T)	5.39
S3 ($^1n\pi^*$-T)	6.74	T4 ($^3\pi_O\pi^*$-T')	5.98
S4 (d)	7.96	T5 (d)	7.96
S5 (d)	8.49	T6 (np)	7.98

Table S3. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $^3n\pi^*$-T' state minimum (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

$^3n\pi^*$-T' state minimum			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0(gs)	1.93	T1 ($^3n\pi^*$-T')	4.46
S1 ($^1n\pi^*$-T')	4.73	T2 ($^3\pi\pi^*$-T')	4.78
S2 ($^1\pi\pi^*$-T')	5.87	T3 ($^3\pi\pi^*$-T)	5.87
S3 ($^1\pi_O\pi^*$-T')	7.28	T4	6.11
S4 (d)	7.77	T5 (d)	7.80
S5 (d)	8.38	T6	8.20

Table S4. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $^1\pi\pi^*$-T' state minimum (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

$^1\pi\pi^*$-T' state minimum			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0 (gs)	1.83	T1 ($^3n\pi^*$-T')	4.68
S1 ($^1\pi\pi^*$-T')	4.69	T2 ($^3\pi\pi^*$-T')	4.98
S2 ($^1n\pi^*$-T')	5.33	T3	5.62
S3	8.16	T4	5.79
S4	8.31	T5	5.86
S5	8.52	T6	8.20

Table S5. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $(ct/\pi\pi*)_{CI}$ (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

$(ct/\pi\pi*)_{CI}$ geometry			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0 (gs)	3.46	T1 ($^3\pi\pi$*-T')	6.43
S1 (ct-$\pi\pi$*-TT')	7.58	T2 ($^3\pi\pi$*-T)	6.49
S2 ($^1\pi\pi$*-T)	7.60	T3 ($^3n\pi$*-T')	7.93
S3 ($^1n\pi$*-T')	7.97	T4 ($^3\pi_O\pi$*-T')	8.13
S4	8.04	T5 (d)	8.60
S5 (d)	8.23	T6 (^{3}ct-$\pi\pi$*-TT')	9.03

Table S6. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $(ct/gs)_{CI\text{-}noreact}$ (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

$(ct/gs)_{CI\text{-}noreact}$ geometry			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0 (ct-$\pi\pi$*-TT')	4.47	T1 (^{3}ct-$\pi\pi$*-TT')	4.43
S1 (gs)	4.53	T2	6.97
S2	7.28	T3	7.03
S3	7.98	T4	7.31
S4	8.50	T5	8.27
S5	9.38	T6	9.18

Table S7. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the $(ct/gs)_{CI\text{-}react}$ (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

$(ct/gs)_{CI\text{-}react}$ geometry			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0 (ct-$\pi\pi$*-TT')	5.02	T1 (^{3}ct-$\pi\pi$*-TT')	5.27
S1 (gs)	5.32	T2	7.94
S2	8.36	T3	8.05
S3	8.75	T4	8.62
S4	9.02	T5	8.66
S5	10.83	T6	8.72

Table S8. CASPT2(12,10)/Amber Calculated Vertical Excitation Energies at the oxe (E_{VA}, eV) for the Lowest Valence Singlet and Triplet Excited States. All energies are reported with respect to the ground state CASPT2(12,10)/Amber energy at the $^1(gs)_{min}$ structure.

oxe geometry			
Singlet states		Triplet states	
State	E_{VA} (eV)	State	E_{VA} (eV)
S0	1.97	T1	5.87
S1	6.02	T2	6.85
S2	6.45	T3	7.24
S3	6.82	T4	7.59
S4	7.46	T5	7.85
S5	8.05	T6	7.87

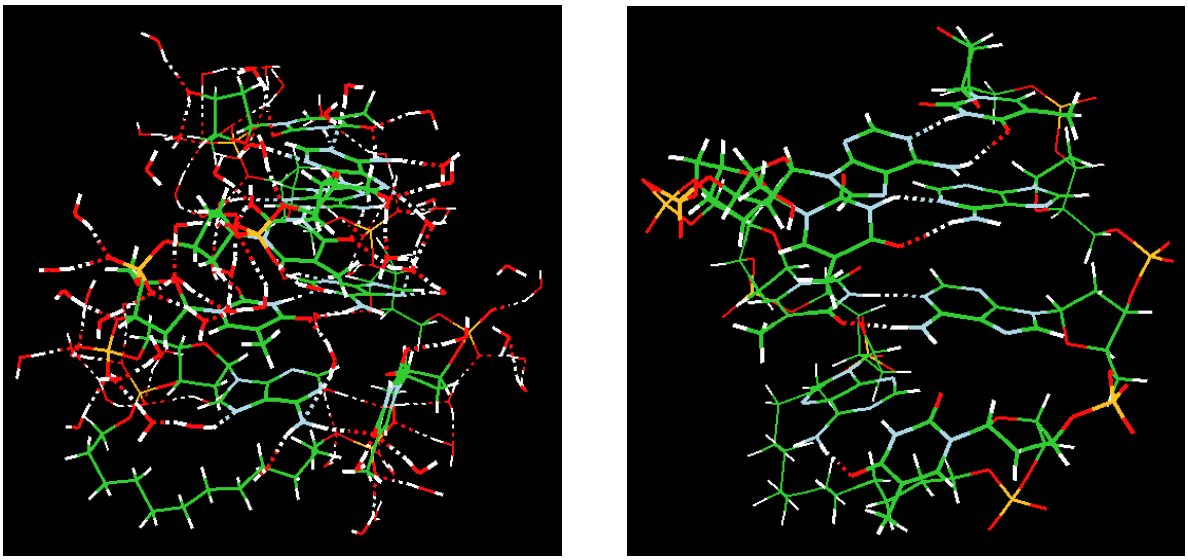
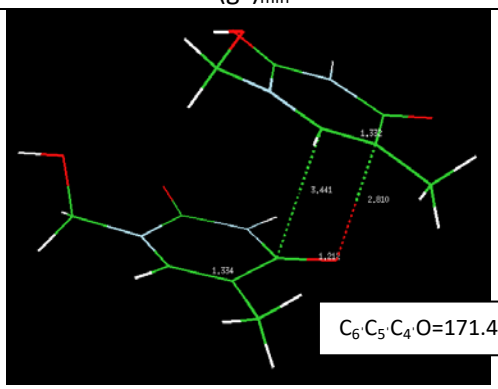
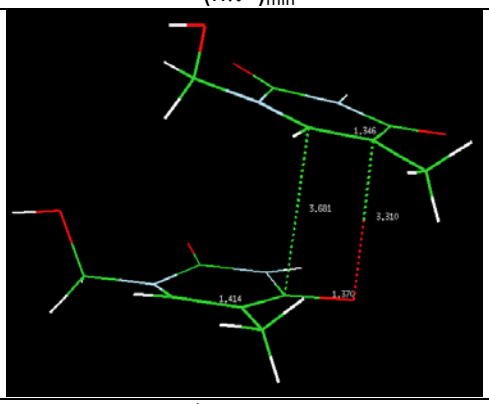
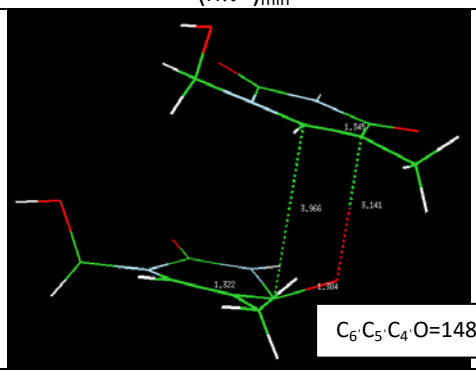
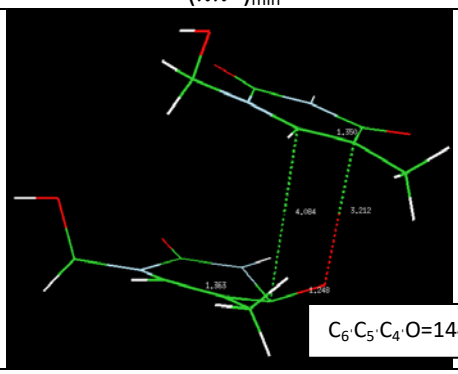
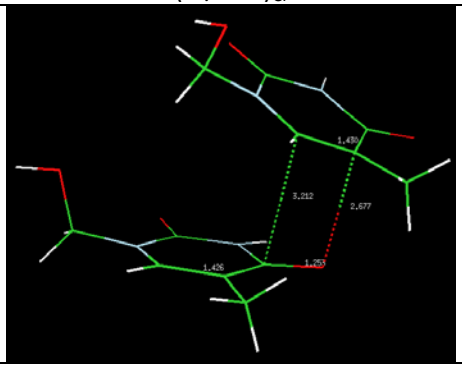
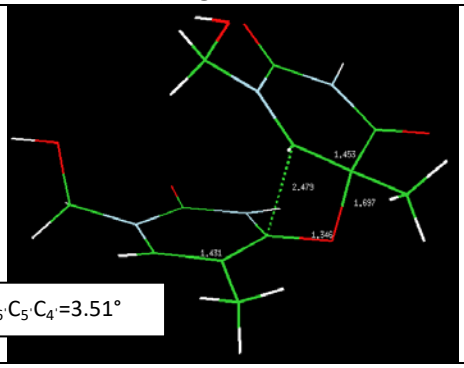


Figure S6. Geometry of the high and medium region of the initial snapshot, with (right) and without (left) water molecules.

$^1(gs)_{min}$	$^1(n\pi^*)_{min}$
 C_6-C_5-C_4-O=171.46°	
$^3(n\pi^*)_{min}$	$^1(\pi\pi^*)_{min}$
 C_6-C_5-C_4-O=148.24°	 C_6-C_5-C_4-O=144.87°
$(ct/\pi\pi^*)_{CI}$	$(ct/gs)_{CI\text{-}noreact}$
	 N_1-C_6-C_5-C_4-=3.51°

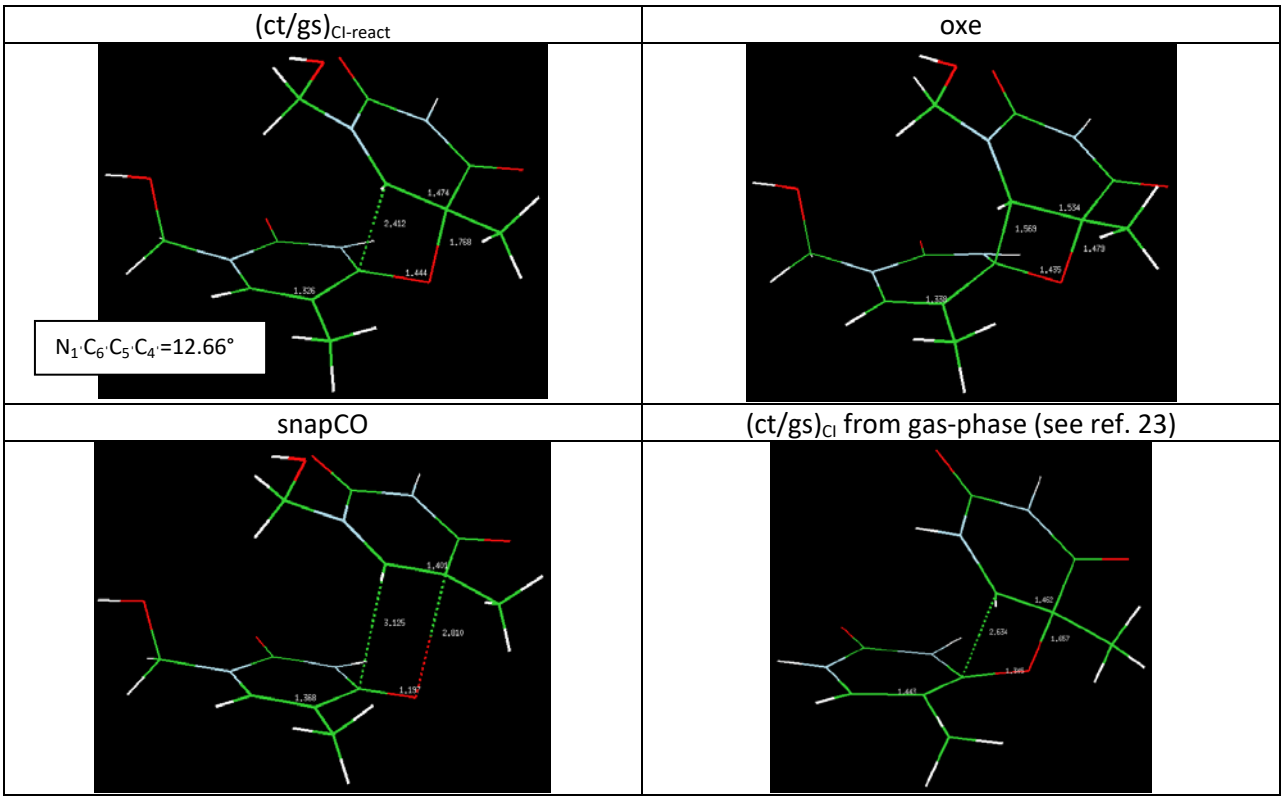


Figure S7. Geometries of the high region of the characterized critical points. Selected intra- and inter-molecular distances are reported in Å.

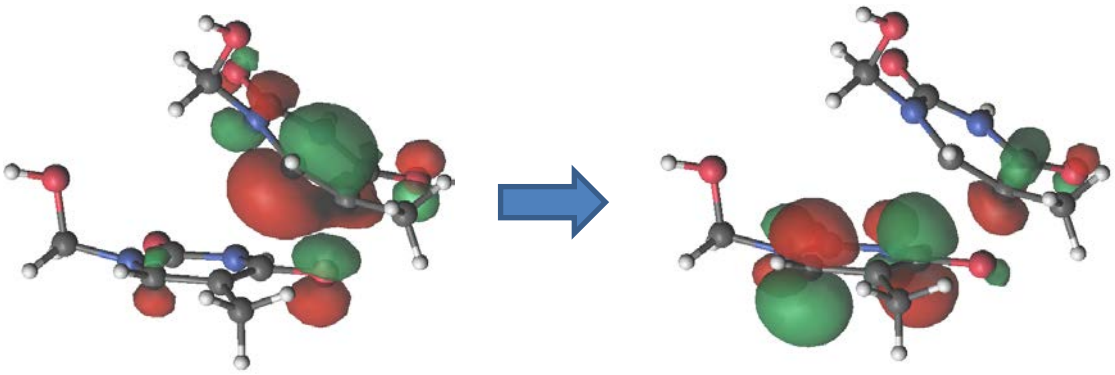


Figure S8. Orbitals mainly describing the singlet at triplet ct-ππ*-TT' states at the $(ct/gs)_{CI\text{-}noreact}$ structure.

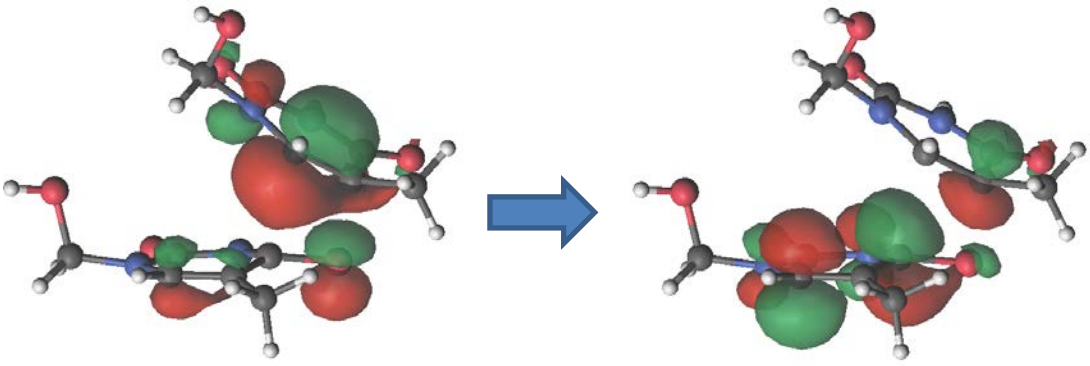


Figure S9. Orbitals mainly describing the singlet and triplet ct-ππ*-TT' states at the $(ct/gs)_{CI\text{-}react}$ structure.

Figure S10. Cartesian coordinates x, y, z (in Å) of the high region of the main discussed structures.

snapCO

O	5.77600003	0.68800000	-4.42100002
C	5.14600003	0.62800000	-3.18100001
H	5.09600002	1.60800001	-2.69100001
N	3.68600002	0.27800000	-3.45100002
C	3.31600001	-0.96200000	-3.81100002
H	4.04600002	-1.72200001	-4.03100002
C	2.03600001	-1.25200001	-4.30100002
C	1.85600001	-2.55200001	-5.17100002
H	1.31600000	-2.31200001	-6.09100003
H	2.83600001	-2.94200002	-5.47100003
H	1.23600000	-3.24200002	-4.60100002
C	1.04600001	-0.10200000	-4.30100002
O	-0.09400000	-0.18200000	-4.75100002
N	1.52600001	1.15800000	-3.91100002
H	0.85600000	1.91800001	-3.85100002
C	2.75600001	1.37800000	-3.32100001
O	3.05600002	2.46800001	-2.89100001
O	5.17600002	0.78800000	0.91900001
C	4.30600002	-0.05200000	1.59900001
H	3.69600002	0.56800000	2.25900001
N	3.49600001	-0.83200000	0.59900000
C	4.02600002	-1.97200001	-0.01100000
H	5.00600002	-2.31200001	0.27900000
C	3.28600002	-2.70200001	-0.90100001
C	3.89600002	-3.91200002	-1.48100000
H	3.46600002	-4.85200002	-1.14100001
H	3.72600001	-3.86200002	-2.56100001
H	4.96600002	-3.89200002	-1.28100001
C	1.95600001	-2.15200001	-1.26100000
O	1.21600001	-2.69200001	-2.03100001
N	1.52600001	-1.05200000	-0.63100000
H	0.56600000	-0.80200000	-0.81100000
C	2.22600001	-0.35200000	0.27900000

O	1.69600001	0.63800000	0.81900000
H	6.70285110	0.66113476	-4.26652484
H	5.71028574	-0.02914286	-2.52385715
H	5.89464541	1.02307093	1.52346809
H	4.87742859	-0.63771429	2.29900001

$^{1}(gs)_{min}$

O	5.66492903	0.80646301	-4.46449002
C	5.04821702	0.67590200	-3.21087901
H	5.02916102	1.61353201	-2.68766401
N	3.67330002	0.26948400	-3.40722202
C	3.35449702	-0.89305600	-4.10904202
H	4.19243802	-1.52746401	-4.32189402
C	2.11930201	-1.23367301	-4.47207402
C	1.78584001	-2.48678701	-5.22861802
H	1.32696201	-2.25139201	-6.18299403
H	2.68031201	-3.06885102	-5.40941303
H	1.08979900	-3.09341501	-4.66501102
C	1.05487700	-0.26321300	-4.22495302
O	-0.08455300	-0.34349200	-4.61134902
N	1.44434000	0.84283401	-3.51420602
H	0.72195200	1.50441701	-3.27063002
C	2.69682401	1.18367000	-3.11517101
O	2.90329201	2.21994501	-2.53715501
O	5.01162803	0.75374101	0.91326000
C	4.20308502	-0.13576200	1.63188501
H	3.51134101	0.39389700	2.26059401
N	3.40510002	-0.92831201	0.71472600
C	3.87945202	-2.03986401	0.03127200
H	4.87281702	-2.35861601	0.26747000
C	3.19183202	-2.72470101	-0.88330100
C	3.69478701	-3.99169202	-1.51859201
H	3.14813201	-4.85234002	-1.14842601
H	3.57741802	-3.96247902	-2.59261901
H	4.74524402	-4.13356602	-1.29871501
C	1.89634301	-2.19314101	-1.27639601
O	1.21493801	-2.60324501	-2.19056301
N	1.48567200	-1.10300300	-0.56539600
H	0.55277900	-0.76757100	-0.75781200
C	2.16780201	-0.41688000	0.39513600
O	1.69475200	0.57051501	0.88677200
H	6.59778918	0.68275122	-4.34488661
H	5.62638702	-0.04102657	-2.63016044
H	5.75415393	0.98214800	1.46055011
H	4.86020716	-0.73053057	2.26246501

$^{1}(n\pi^{*})_{min}$

O	5.72575603	0.87834500	-4.44536302
C	5.06919602	0.71794600	-3.22844602
H	5.01358002	1.64591101	-2.67804301
N	3.71228502	0.30064900	-3.46699202
C	3.43910302	-0.88134200	-4.16161102

H	4.28217502	-1.52140601	-4.32461002
C	2.20868801	-1.22091400	-4.58918702
C	1.90798201	-2.51885801	-5.26710302
H	1.36042900	-2.36141201	-6.18533103
H	2.82497301	-3.04409801	-5.49678803
H	1.30304801	-3.15702201	-4.63580002
C	1.11355501	-0.28553900	-4.32080502
O	-0.02726900	-0.44332300	-4.66852402
N	1.46860901	0.82774500	-3.62513102
H	0.73566200	1.47378301	-3.37174601
C	2.71976701	1.19456301	-3.21945701
O	2.89058802	2.24838101	-2.67717001
O	5.10060602	0.81676601	0.95442700
C	4.25048302	-0.06593000	1.64625201
H	3.56499902	0.48635000	2.26421601
N	3.48211702	-0.83929800	0.72621001
C	4.03331402	-1.94323201	0.03165700
H	5.08078302	-2.12145201	0.11160900
C	3.21939302	-2.71825101	-0.82647701
C	3.71848101	-3.99219002	-1.45578801
H	3.26119501	-4.86276902	-0.99619701
H	3.51466902	-4.01987602	-2.52013801
H	4.79097002	-4.06514602	-1.33026401
C	2.01599801	-2.22045101	-1.04226501
O	1.08957900	-2.77126901	-1.88787501
N	1.57549900	-1.02660901	-0.53253100
H	0.62625400	-0.73776400	-0.67305100
C	2.30941101	-0.29764300	0.35002300
O	1.88215701	0.74089001	0.73400500
H	6.65204427	0.72658053	-4.31077551
H	5.63773460	0.00545600	-2.62163101
H	5.85108069	0.99867799	1.50435125
H	4.87672802	-0.68294286	2.28741415

$^3(n\pi^*)_{min}$

O	5.70506703	0.85994700	-4.44321102
C	5.06738602	0.69082801	-3.21661802
H	5.04139702	1.61642101	-2.66106201
N	3.70899602	0.28278100	-3.42339802
C	3.41319501	-0.87745900	-4.13634102
H	4.24042202	-1.53998501	-4.29069802
C	2.18170101	-1.18197001	-4.58402602
C	1.84547001	-2.47334801	-5.25320802
H	1.33680201	-2.31046901	-6.19254203
H	2.74477101	-3.04486501	-5.43961402
H	1.18989601	-3.06737701	-4.63044802
C	1.11861601	-0.21546700	-4.31299502
O	-0.02833500	-0.34218500	-4.65101702
N	1.51397400	0.89350800	-3.63555002
H	0.79262501	1.55556901	-3.39873801
C	2.76570701	1.23569700	-3.22926501
O	2.97783501	2.29271001	-2.74113201
O	5.11650202	0.81782501	0.92634900
C	4.25947902	-0.06327700	1.60552301
H	3.56222202	0.48307300	2.21618001

N	3.48517702	-0.83770100	0.67215100
C	4.01369302	-1.93981601	-0.02213100
H	5.06522302	-2.10868201	0.08876600
C	3.28141801	-2.75456401	-0.76281200
C	3.80622301	-3.98701502	-1.44088901
H	3.30495601	-4.87228202	-1.05874001
H	3.64813602	-3.95102002	-2.51291501
H	4.87022702	-4.08536402	-1.27057400
C	1.86396401	-2.44401801	-0.83809900
O	1.27374101	-2.78825401	-2.04157401
N	1.51087701	-1.14636000	-0.46788500
H	0.55967400	-0.85197500	-0.60331800
C	2.23996501	-0.36228900	0.35299900
O	1.79908201	0.68320600	0.75170700
H	6.63394441	0.71175225	-4.32064840
H	5.64476888	-0.02727914	-2.62596658
H	5.85967539	0.99873626	1.48622615
H	4.87629045	-0.68336700	2.25378016

$^1(\pi\pi^*)_{min}$

O	5.74097302	0.86351000	-4.49178802
C	5.07761702	0.72488800	-3.25722702
H	5.04719203	1.66469701	-2.73742301
N	3.70961001	0.32366300	-3.49143102
C	3.40408102	-0.86129100	-4.18316502
H	4.23130702	-1.52321200	-4.33796002
C	2.16201101	-1.18205600	-4.60348902
C	1.81623501	-2.48468301	-5.26355802
H	1.29098600	-2.32014301	-6.19795503
H	2.71440601	-3.05621302	-5.46219302
H	1.17415801	-3.06387401	-4.61068902
C	1.09286000	-0.21288600	-4.34864802
O	-0.04411100	-0.31956800	-4.71881602
N	1.47906900	0.89705801	-3.65578601
H	0.75726600	1.55871201	-3.41133501
C	2.73101501	1.23877200	-3.24767901
O	2.91863701	2.29187501	-2.69941701
O	5.07907402	0.74057100	0.93963900
C	4.25465702	-0.14722700	1.64163301
H	3.54977602	0.38223900	2.25653201
N	3.47650201	-0.94421300	0.71207901
C	3.99171902	-1.97009501	-0.00337800
H	5.02786602	-2.20862201	0.14556900
C	3.24237701	-2.81533001	-0.76664800
C	3.78308902	-3.94975002	-1.52033001
H	3.25661101	-4.84815602	-1.20167700
H	3.58986602	-3.84345802	-2.57914601
H	4.84790602	-4.06023002	-1.37332100
C	1.67374601	-2.52618101	-0.87919100
O	1.20470500	-2.80435601	-2.00157001
N	1.48045600	-1.17957300	-0.47611400
H	0.57998700	-0.79852700	-0.71979600
C	2.18820901	-0.45245300	0.38842700
O	1.80901901	0.58401200	0.84025200

H	6.66619673	0.71259917	-4.35076562
H	5.64094846	0.00793657	-2.65871201
H	5.82476735	0.94883981	1.48795133
H	4.89333131	-0.75059986	2.28208872

$(ct/\pi\pi^*)_{Cl}$

O	5.66492903	0.80646301	-4.46449002
C	5.04821702	0.67590200	-3.21087901
H	5.02916102	1.61353201	-2.68766401
N	3.67330002	0.26948400	-3.40722202
C	3.35449702	-0.89305600	-4.10904202
H	4.19243802	-1.52746401	-4.32189402
C	2.11930201	-1.23367301	-4.47207402
C	1.78584001	-2.48678701	-5.22861802
H	1.32696201	-2.25139201	-6.18299403
H	2.68031201	-3.06885102	-5.40941303
H	1.08979900	-3.09341501	-4.66501102
C	1.05487700	-0.26321300	-4.22495302
O	-0.08455300	-0.34349200	-4.61134902
N	1.44434000	0.84283401	-3.51420602
H	0.72195200	1.50441701	-3.27063002
C	2.69682401	1.18367000	-3.11517101
O	2.90329201	2.21994501	-2.53715501
O	5.01162803	0.75374101	0.91326000
C	4.20308502	-0.13576200	1.63188501
H	3.51134101	0.39389700	2.26059401
N	3.40510002	-0.92831201	0.71472600
C	3.87945202	-2.03986401	0.03127200
H	4.87281702	-2.35861601	0.26747000
C	3.19183202	-2.72470101	-0.88330100
C	3.69478701	-3.99169202	-1.51859201
H	3.14813201	-4.85234002	-1.14842601
H	3.57741802	-3.96247902	-2.59261901
H	4.74524402	-4.13356602	-1.29871501
C	1.89634301	-2.19314101	-1.27639601
O	1.21493801	-2.60324501	-2.19056301
N	1.48567200	-1.10300300	-0.56539600
H	0.55277900	-0.76757100	-0.75781200
C	2.16780201	-0.41688000	0.39513600
O	1.69475200	0.57051501	0.88677200
H	6.59778918	0.68275122	-4.34488661
H	5.62638702	-0.04102657	-2.63016044
H	5.75415393	0.98214800	1.46055011
H	4.86020716	-0.73053057	2.26246501

$(ct/gs)_{Cl\text{-}noreact}$

O	5.66492903	0.80646301	-4.46449002
C	5.04821702	0.67590200	-3.21087901
H	5.02916102	1.61353201	-2.68766401
N	3.67330002	0.26948400	-3.40722202
C	3.35449702	-0.89305600	-4.10904202
H	4.19243802	-1.52746401	-4.32189402
C	2.11930201	-1.23367301	-4.47207402

C	1.78584001	-2.48678701	-5.22861802
H	1.32696201	-2.25139201	-6.18299403
H	2.68031201	-3.06885102	-5.40941303
H	1.08979900	-3.09341501	-4.66501102
C	1.05487700	-0.26321300	-4.22495302
O	-0.08455300	-0.34349200	-4.61134902
N	1.44434000	0.84283401	-3.51420602
H	0.72195200	1.50441701	-3.27063002
C	2.69682401	1.18367000	-3.11517101
O	2.90329201	2.21994501	-2.53715501
O	5.01162803	0.75374101	0.91326000
C	4.20308502	-0.13576200	1.63188501
H	3.51134101	0.39389700	2.26059401
N	3.40510002	-0.92831201	0.71472600
C	3.87945202	-2.03986401	0.03127200
H	4.87281702	-2.35861601	0.26747000
C	3.19183202	-2.72470101	-0.88330100
C	3.69478701	-3.99169202	-1.51859201
H	3.14813201	-4.85234002	-1.14842601
H	3.57741802	-3.96247902	-2.59261901
H	4.74524402	-4.13356602	-1.29871501
C	1.89634301	-2.19314101	-1.27639601
O	1.21493801	-2.60324501	-2.19056301
N	1.48567200	-1.10300300	-0.56539600
H	0.55277900	-0.76757100	-0.75781200
C	2.16780201	-0.41688000	0.39513600
O	1.69475200	0.57051501	0.88677200
H	6.59778918	0.68275122	-4.34488661
H	5.62638702	-0.04102657	-2.63016044
H	5.75415393	0.98214800	1.46055011
H	4.86020716	-0.73053057	2.26246501

$(ct/gs)_{Cl\text{-}react}$

O	5.63437902	0.71174000	-4.41520202
C	5.02948303	0.63097800	-3.17945601
H	5.02678402	1.59326401	-2.68717601
N	3.66622002	0.21539100	-3.28153101
C	3.34715102	-1.12988900	-3.59885302
H	4.13743902	-1.70340501	-4.03570502
C	1.97186801	-1.54956901	-3.92458502
C	1.78978401	-2.58903901	-4.99816702
H	1.45825400	-2.11973701	-5.91521803
H	2.71475801	-3.11299702	-5.18729102
H	1.02643800	-3.29962901	-4.70048302
C	1.00256200	-0.35378400	-4.04460002
O	-0.05219400	-0.44830000	-4.54771602
N	1.46490901	0.80243900	-3.55585501
H	0.78467400	1.55067000	-3.45884602
C	2.75544001	1.19070001	-3.18126501
O	2.93581301	2.27332901	-2.84776201
O	5.06707802	0.77770100	0.91267800
C	4.20036702	-0.12308100	1.57101201
H	3.48690801	0.42346900	2.17731901
N	3.44306001	-0.86030400	0.60319601

C	3.93467702	-1.99517701	-0.10064400
H	4.92241402	-2.29938301	0.15738800
C	3.28123601	-2.58271101	-1.09385600
C	3.72639802	-3.91315802	-1.63296901
H	3.23250202	-4.69596302	-1.06663600
H	3.48301001	-4.05683002	-2.67860501
H	4.78573102	-4.02636102	-1.51128201
C	2.21355601	-1.89551101	-1.61172201
O	1.24067000	-2.39582801	-2.55481401
N	1.65726901	-0.86808800	-0.87598200
H	0.74521500	-0.57896500	-1.07548100
C	2.26035001	-0.32903400	0.20540000
O	1.72036801	0.61093701	0.76958701
H	6.57823512	0.63397921	-4.29357162
H	5.64153517	-0.03996914	-2.55403387
H	5.80666286	0.95742884	1.46550437
H	4.81612631	-0.72917243	2.23633058

oxe

O	5.52600003	0.63032800	-4.39398402
C	4.95806102	0.58719700	-3.12485501
H	4.95502302	1.56438201	-2.66764501
N	3.58360401	0.17477700	-3.20251501
C	3.13474601	-1.18225300	-3.19001901
H	3.92298302	-1.84157901	-3.51118102
C	1.82752201	-1.56490001	-3.89537702
C	1.83230001	-2.47738001	-5.10414102
H	1.72363601	-1.92113801	-6.02743003
H	2.74229001	-3.06279601	-5.13959702
H	0.98489900	-3.14873802	-5.02234902
C	0.91234300	-0.35902300	-4.08314202
O	-0.16170500	-0.41561200	-4.60328702
N	1.38896101	0.81659600	-3.61526001
H	0.72823600	1.57578501	-3.54621702
C	2.66532401	1.16201000	-3.23181202
O	2.89712602	2.30577901	-2.99461402
O	5.04697403	0.80283400	0.92630101
C	4.22657002	-0.11962300	1.59236301
H	3.51201302	0.38949700	2.20659901
N	3.48327002	-0.88526301	0.61622100
C	3.87917702	-2.09446901	0.03763400
H	4.62340602	-2.67223101	0.54486800
C	3.35889901	-2.61870501	-1.07765901
C	3.71167302	-3.99268102	-1.57938301
H	3.11310202	-4.75323902	-1.09185701
H	3.54997802	-4.08392402	-2.64444301
H	4.75647502	-4.20038902	-1.39423201
C	2.46172001	-1.71350401	-1.87636001
O	1.42690701	-2.30136201	-2.67733001
N	1.84634401	-0.76926900	-1.01344800
H	0.88396600	-0.53345700	-1.17705600
C	2.32900401	-0.29640100	0.15527000
O	1.76581601	0.58685200	0.74140900
H	6.46908912	0.59599287	-4.28799994

```
H       5.59161603  -0.05877371  -2.51097787
H       5.79973224   0.98954211   1.47540855
H       4.87092431  -0.72468300   2.22826587
```