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

Supporting Information

Mechanisms and Energetics for Benzophenone Photosensitized Thymine Damage and Repair from Paternò-Büchi Cycloaddition

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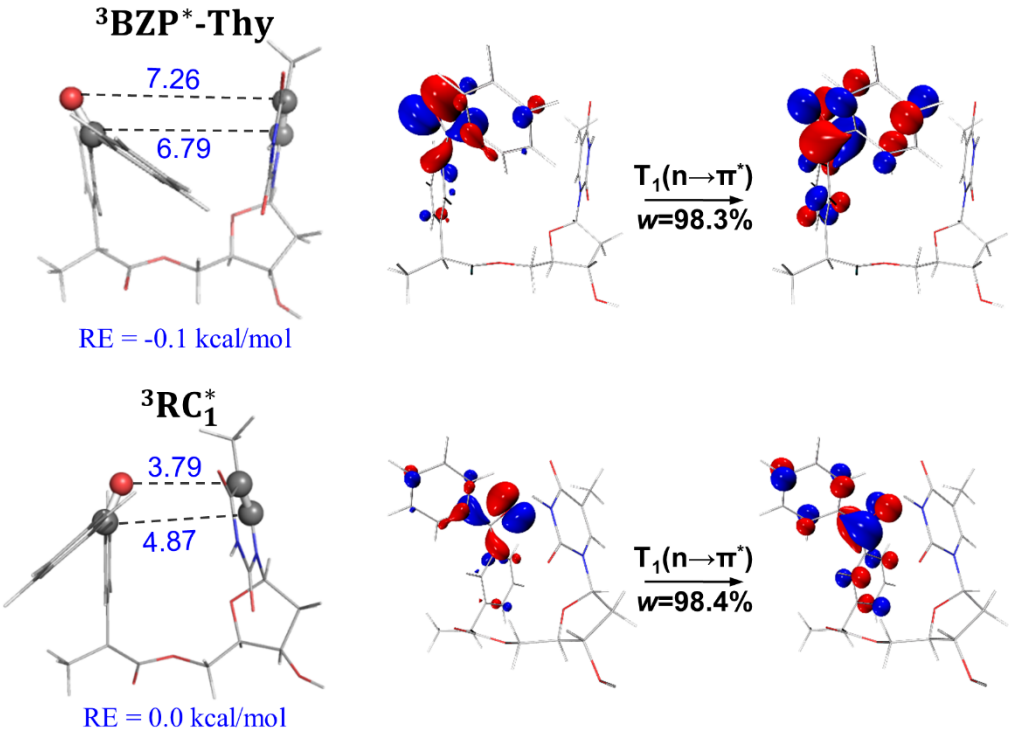


Figure S1. The optimized geometries of ^{3}BZP*-Thy and ^{3}RC$_1^*$ and their main hole and electron natural transition orbitals (NTO, isovalue = 0.05 e·Å^{-3}) for T_1 excited states. RE stand for the T_1 energies relative to ^{3}RC$_1^*$. The bond lengths of C1-C4 and O2-C3 are marked (Units in Å). The color of the atoms in white, grey, blue and red stand for hydrogen, carbon, nitrogen and oxygen, respectively.

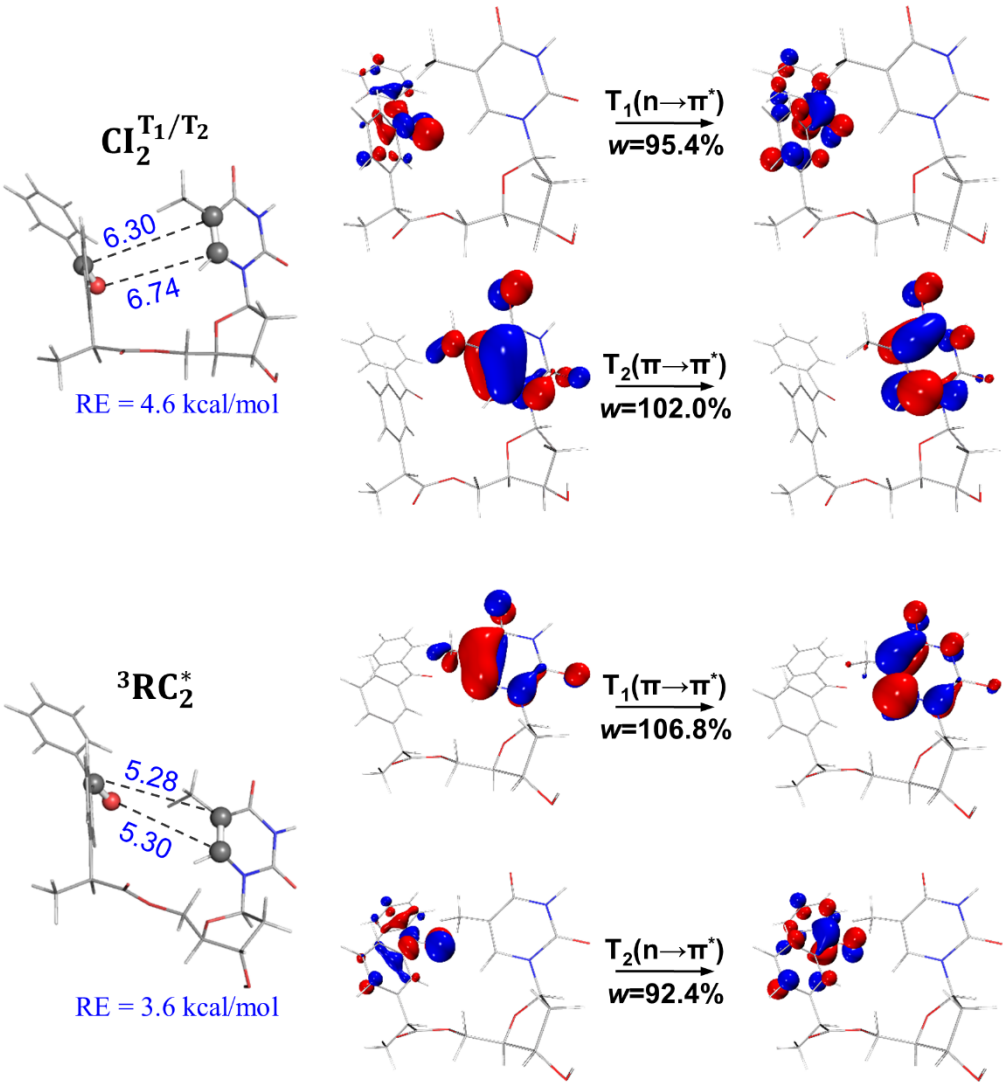


Figure S2. The optimized geometries of $CI_2^{T_1/T_2}$ and $^3RC_2^*$ and their main hole and electron NTO (Isovalue = 0.05 e·Å^{-3}) for T_1 and T_2 excited states. RE stand for the T_1 energies relative to $^3RC_1^*$. The bond lengths of C1-C3 and O2-C4 are marked (Units in Å). The color of the atoms in white, grey, blue and red stand for hydrogen, carbon, nitrogen and oxygen, respectively.

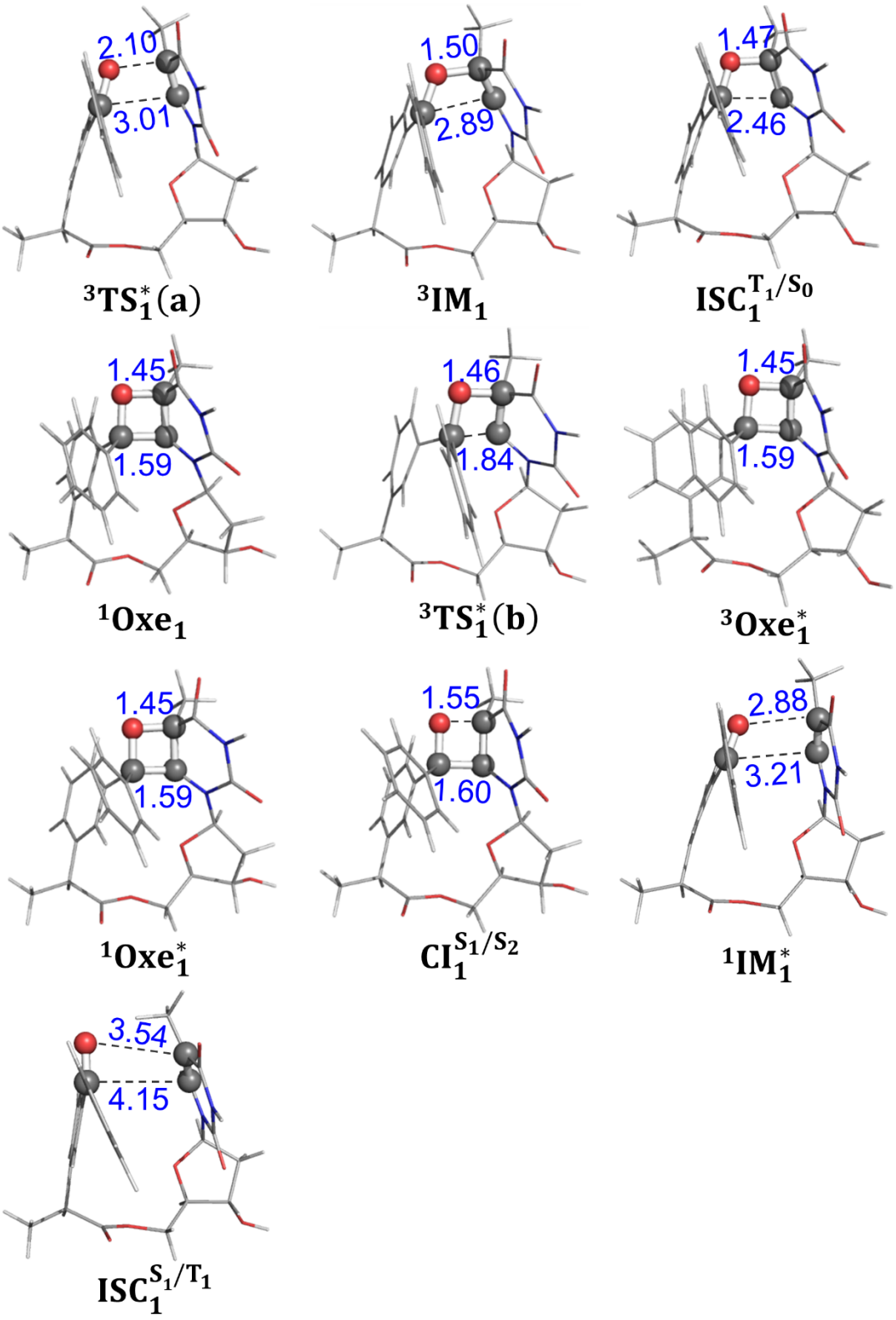


Figure S3. The optimized geometries of the head-to-head Paternò-Büchi cycloaddition and corresponding photoinduced cycloreversion with the bond lengths of C1-C4 and O2-C3 (Units in Å).

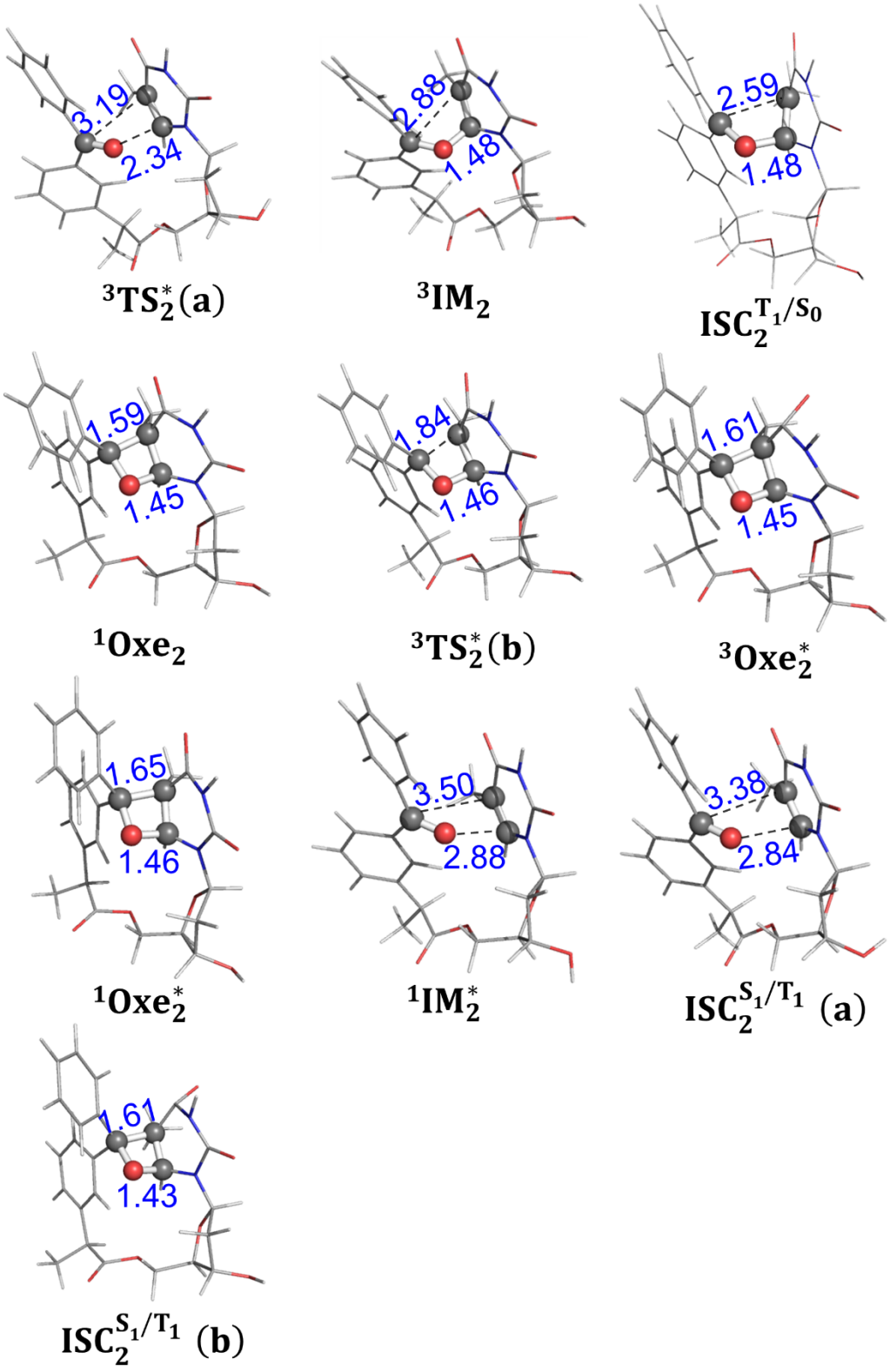


Figure S4. The optimized geometries of the head-to-tail Paternò-Büchi cycloaddition and corresponding photoinduced cycloreversion with the bond lengths of C1-C3 and O2-C4 (Units in Å).

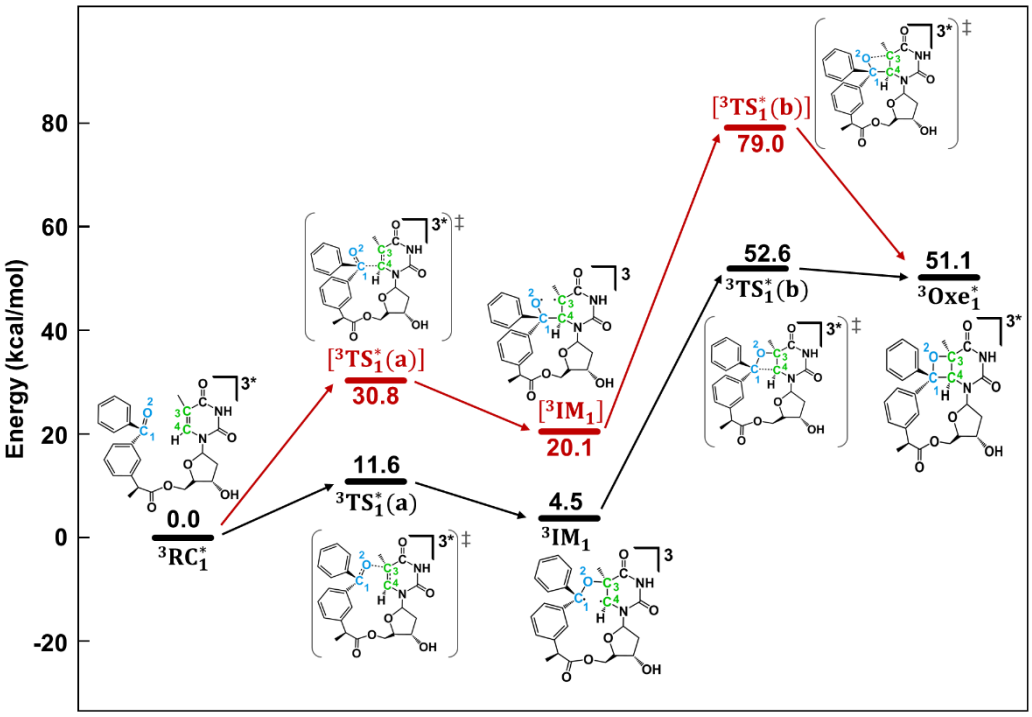


Figure S5. Reaction pathways and potential energy profiles of PB cycloaddition for BZP-Thy in acetonitrile in the head-to-head form. The red and black lines represent the paths for the first formation of C1-C4 bond and O2-C3 bond, respectively. The energy is relative to the T_1 state energy of $^3RC_1^*$.

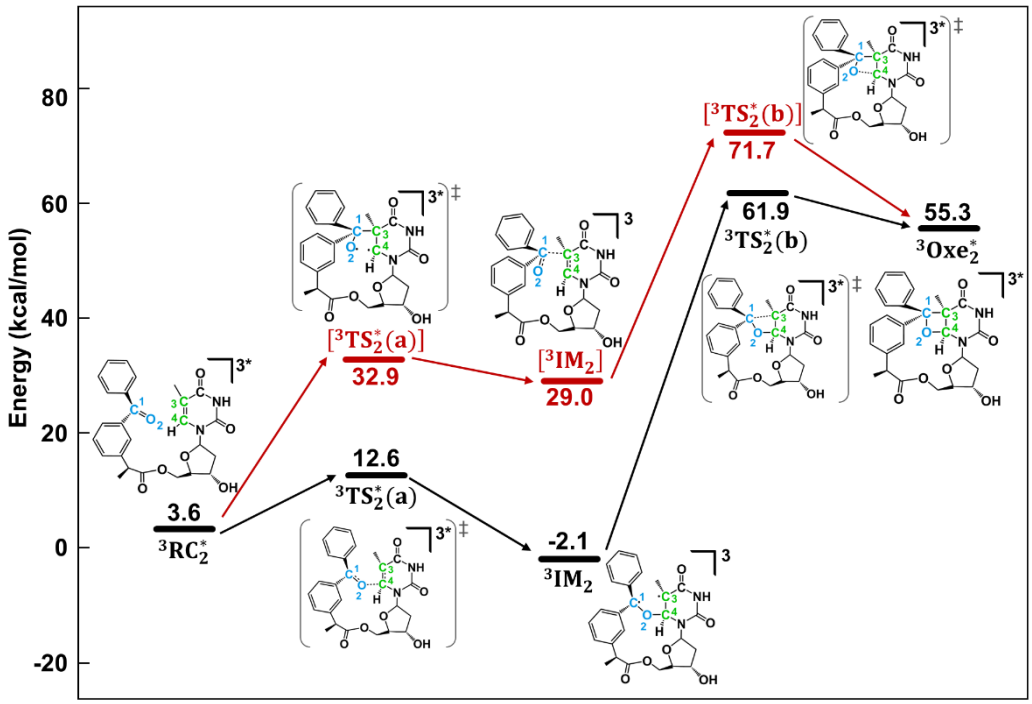


Figure S6. Reaction pathways and potential energy profiles of PB cycloaddition for BZP-Thy in acetonitrile in the head-to-tail form. The red and black lines represent the paths for the first formation of C1-C3 bond and O2-C4 bond, respectively. The energy is relative to the T_1 state energy of $^3RC_1^*$.

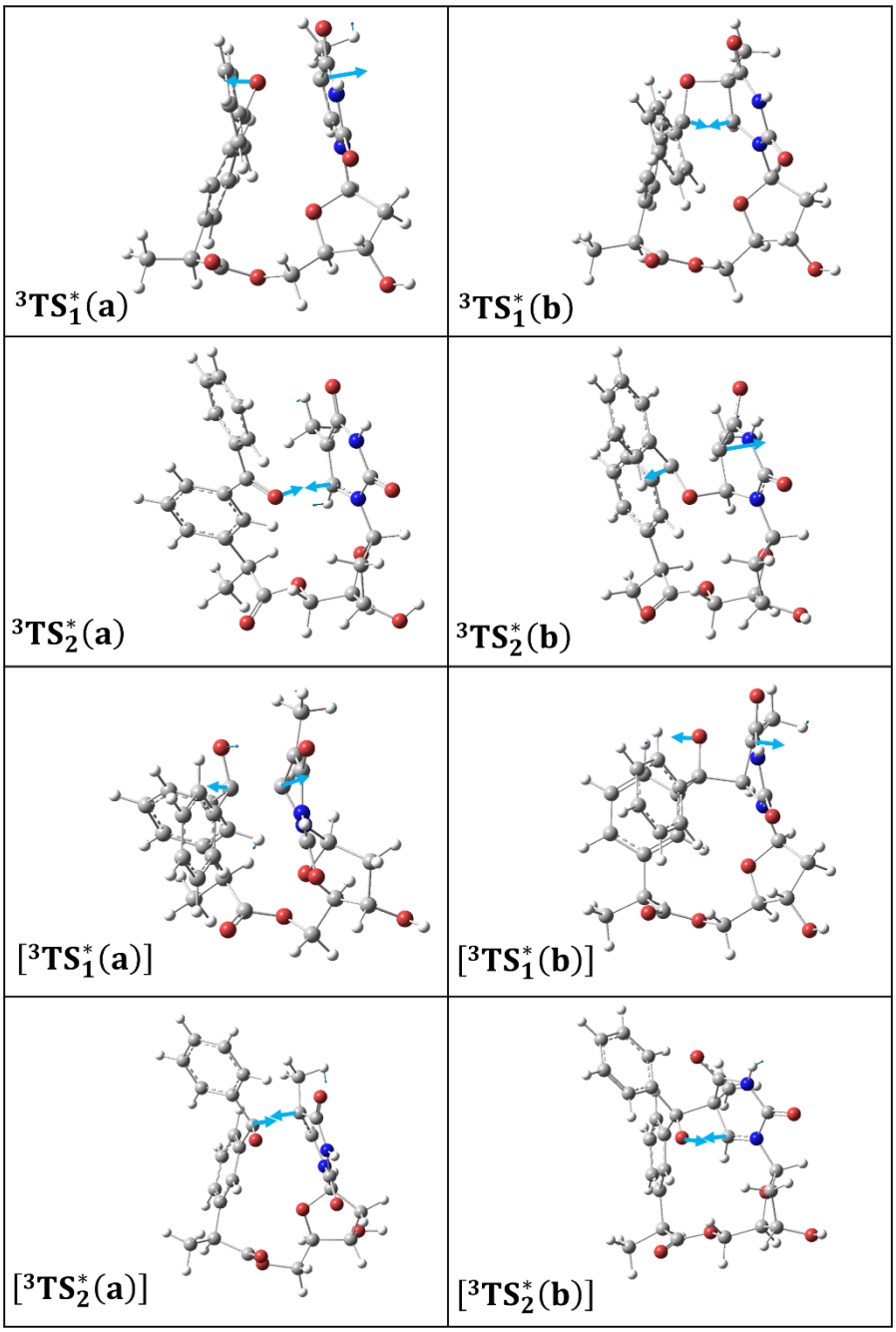


Figure S7. Schematic diagram of the vibrational motion along the unique imaginary frequency (v) for each transition state.

Supplementary Tables

Table S1. The unique imaginary frequency (cm^{-1}) for each transition state.

Transition state	Imaginary frequency
$^{3}TS^{*}_{1}$(a)	-213.42
$^{3}TS^{*}_{1}$(b)	-778.80
$^{3}TS^{*}_{2}$(a)	-162.35
$^{3}TS^{*}_{2}$(b)	-1269.33
$\overline{^{3}TS^{*}_{1}(a)}$	-304.72
$\overline{^{3}TS^{*}_{1}(b)}$	-425.82
$\overline{^{3}TS^{*}_{2}(a)}$	-420.15
$\overline{^{3}TS^{*}_{2}(b)}$	-643.33

Table S2. The spin orbit coupling (SOC in cm^{-1}) in the optimized ISC regions.

ISC process	SOC
$^{3}IM_{1}\rightarrow{}^{1}Oxe_{1}$	3.14
$^{1}Oxe^{*}_{1}\rightarrow{}^{3}Oxe^{*}_{1}$	0.81[a]
$^{1}IM^{*}_{1}\rightarrow{}^{3}RC^{*}$	0.84
$^{3}IM_{2}\rightarrow{}^{1}Oxe_{2}$	4.65
$^{1}Oxe^{*}_{2}\rightarrow{}^{3}Oxe^{*}_{2}$	0.70
$^{1}IM^{*}_{2}\rightarrow{}^{3}RC^{*}$	2.40

[a] From the ISC starting reactant $^{1}Oxe^{*}_{1}$.

Table S3 The main hole and electron NTO (Isovalue = 0.05 e·Å^{-3}) of T_1 excited states along with the IRC (amu$^{1/2}$bohr) on the reactant side of $^{3}TS^{*}_{1}(a)$. The IRC of $^{3}TS^{*}_{1}(a)$ is 0.00 amu$^{1/2}$bohr.

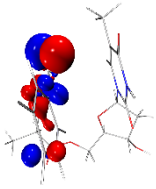
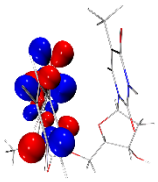
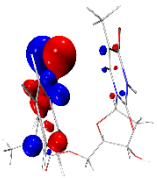
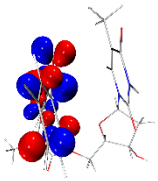
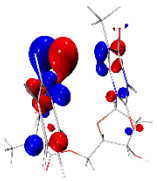
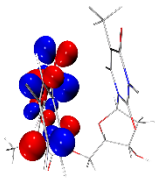
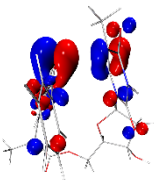
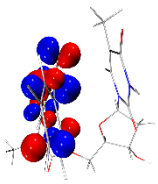
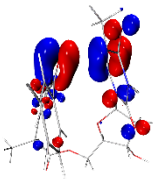
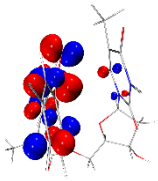
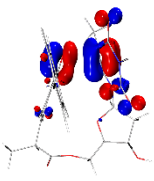
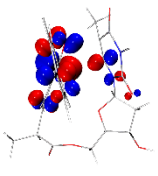
IRC	Hole-NTO	Electron-NTO
-6.24		
-5.03		
-3.78		
-2.52		
-1.26		
0.00 ($^{3}TS^{*}_{1}(a)$)		

Table S4. The main hole and electron NTO (Isovalue = 0.05 e·Å^{-3}) of T_1 and T_2 excited states along with the IRC (amu$^{1/2}$bohr) on the reactant side $^{3}TS_{2}^{*}(a)$. The IRC of $^{3}TS_{2}^{*}(a)$ is 0.00 amu$^{1/2}$bohr.

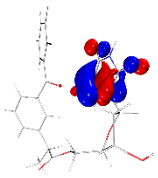
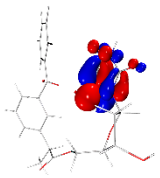
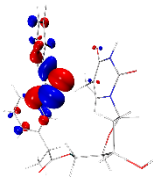
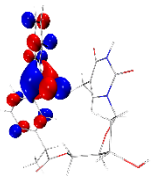
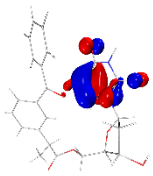
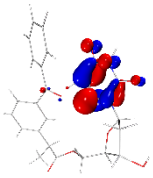
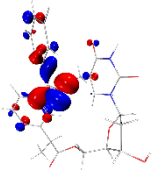
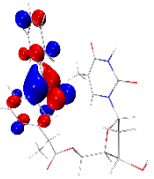
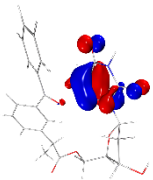
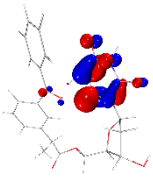
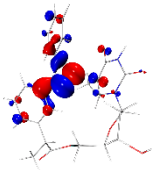
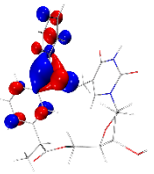
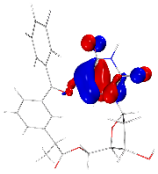
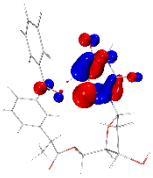
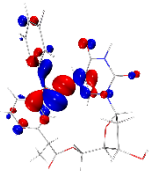
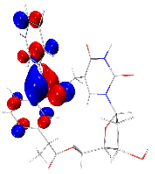
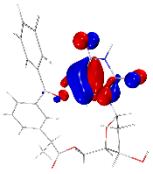
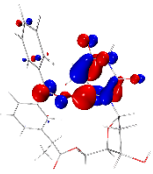
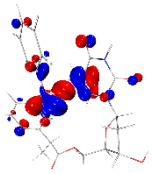
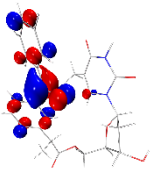
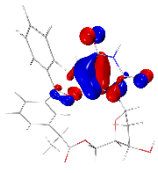
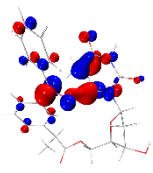
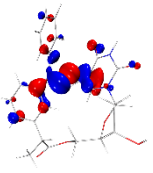
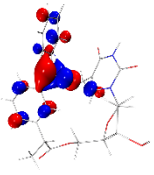
IRC	T_1		T_2	
	Hole-NTO	Electron-NTO	Hole-NTO	Electron-NTO
-5.43				
-4.37				
-3.36				
-2.25				
-1.12				
0.00 ($^{3}TS_{2}^{*}(a)$)				

Table S5. Relative energy (RE in kcal/mol), vertical excitation energy (ΔE in eV), absorption wavelength (λ in nm), oscillator strength f, solvent reorganization energy (SRE in eV) and dipole moment (μ in Debye) of main excited states for the $^{1}Oxe_{1}$ and $^{1}Oxe_{2}$ geometries. The reference energy is the T_1 state energy of $^{3}RC^{*}_{1}$.

Geometry	State	RE	ΔE	λ	f	SRE	μ
$^{1}Oxe_{1}$	S_0	-34.3					6.64
	S_1	77.3	4.8444	256	0.0014	0.02	5.52
	S_2	84.0	5.1365	241	0.0375	0.08	10.36
	S_3	86.0	5.2232	237	0.0045	0.17	12.38
	S_4	87.2	5.2743	235	0.0167	0.01	7.39
	S_5	91.0	5.4384	228	0.0051	0.12	8.19
$^{1}Oxe_{2}$	S_0	-34.4					2.77
	S_1	73.7	4.6913	264	0.0044	0.22	12.64
	S_2	77.9	4.8716	255	0.0016	0.24	12.47
	S_3	88.4	5.3284	233	0.0038	0.03	5.05
	S_4	89.8	5.3866	230	0.0113	0.07	9.65
	S_5	90.8	5.4315	228	0 .0315	0.16	13.57

The excited-state properties in Table S5 were obtained through the self-consistent state-specific TD-B3LYP/IEFPCM method using Q-Chem 5.4 package. The lowest excited states (S_1) with small oscillator strengths are located at 256 nm and 264 nm for $^{1}Oxe_{1}$ and $^{1}Oxe_{2}$, respectively. Combined with the NTO distributions in Table S6, the S_1 states of $^{1}Oxe_{1}$ and $^{1}Oxe_{2}$ were naturally attributed to the $n\rightarrow\pi^{*}$ local transition and the $\pi\rightarrow\pi^{*}$ charge-transfer transition, respectively. The photoexcited bright states with largest oscillator strengths for $^{1}Oxe_{1}$ and $^{1}Oxe_{2}$ are located at ca. 241 nm (S_2) and 228 nm (S_5). Both of the high excited states are attributed to the $\pi\rightarrow\pi^{*}$ transition, but the charge-transfer characteristic of $^{1}Oxe_{2}$ is more obvious than that of $^{1}Oxe_{1}$. The charge-transfer excited states of $^{1}Oxe_{2}$ possess the large dipole moments and solvent reorganization energies, which emphasizes the significance of solvation effect on the regio-isomerism of vertical excitation processes for head-to-head and head-to-tail oxetanes in acetonitrile.

Table S6. The main hole and electron NTO (Isovalue = 0.05 e·Å^{-3}) for photoexcited bright states of $^{1}Oxe_1$ and $^{1}Oxe_2$. *w* denotes the square of the singular value for a given NTO pair, i.e. the associated weight for each NTO pair.

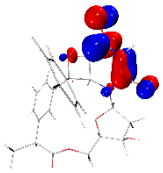
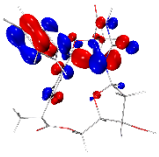
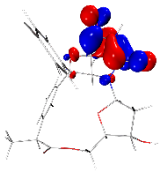
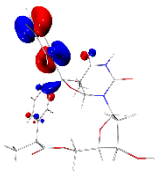
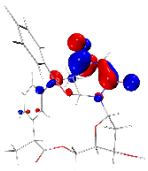
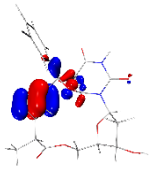
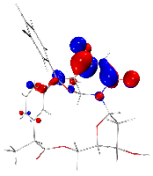
Geometry	Excited State	Nature	*w*	Hole-NTO	Electron-NTO
$^{1}Oxe_1$	S_1	$^{1}(n\pi^*)$	99.2%		
	S_2	$^{1}(\pi\pi^*)$	97.4%		
$^{1}Oxe_2$	S_1	$^{1}(\pi\pi^*)$	99.5%		
	S_5	$^{1}(\pi\pi^*)$	91.2%		

Table S7. The main hole and electron NTO (Isovalue = 0.05 e·Å^{-3}) for S_1 and S_2 excited states of $^{CI}{}_{1}^{S_1/S_2}$. *w* denotes the square of the singular value for a given NTO pair, i.e. the associated weight for each NTO pair.

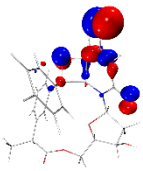
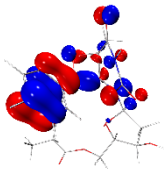
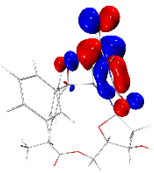
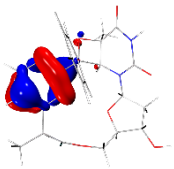
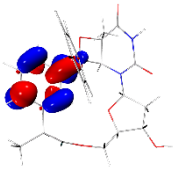
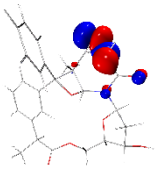
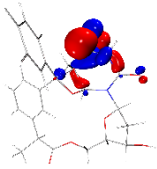
Excited State	Nature	*w*	Hole-NTO	Electron-NTO
S_1	$^1(n\pi^*)$	99.6%		
S_2	$^1(\pi\pi^*)$	99.8%		

Table S8. The main hole and electron NTO (Isovalue = 0.05 e·Å^{-3}) for T_1 excited states of $^3Oxe^*_1$ and $^3Oxe^*_2$. *w* denotes the square of the singular value for a given NTO pair, i.e. the associated weight for each NTO pair.

Geometry	Nature	*w*	Hole-NTO	Electron-NTO
$^3Oxe^*_1$	$^3(\pi\pi^*)$	108.7%		
$^3Oxe^*_2$	$^3(\pi\pi^*)$	101.9%		

Cartesian Coordinates

^{3}BZP*-Thy				^{3}RC$_1^*$			
C	-4.630111	2.963284	-0.081413	C	-0.665646	5.007428	-0.169188
H	-5.390154	2.918659	0.704347	H	-1.174907	5.527750	0.647630
H	-4.642515	3.966909	-0.519129	H	-0.115311	5.746117	-0.761029
H	-4.894572	2.245064	-0.862514	H	-1.421211	4.549216	-0.813553
O	-0.949886	2.911126	-0.023371	O	2.125835	2.597741	-0.241004
C	0.165041	2.870337	-0.943064	C	2.796499	1.676194	-1.130279
H	0.178655	1.903941	-1.453049	H	2.053962	1.133392	-1.717883
H	0.055338	3.667694	-1.684521	H	3.455626	2.235395	-1.802776
O	1.634831	1.966429	0.737671	O	2.714487	-0.018538	0.570089
C	2.682982	3.141987	-1.060955	C	4.392015	-0.305359	-1.120476
C	3.771362	2.465631	-0.207997	C	4.258792	-1.609197	-0.309487
H	2.515324	2.570850	-1.978423	H	3.929805	-0.425576	-2.103790
H	4.327985	3.244693	0.321774	H	5.156577	-1.722465	0.305964
H	4.477502	1.877167	-0.796298	H	4.155096	-2.496761	-0.935491
O	2.930975	4.510705	-1.359126	O	5.727742	0.169380	-1.251379
H	3.543966	4.542885	-2.110113	H	6.150461	-0.335513	-1.963633
N	3.136582	0.145235	0.665045	N	1.841077	-2.197273	0.317411
C	2.758830	-0.459470	-0.529334	C	1.271029	-2.138859	-0.950672
O	2.356138	0.159530	-1.509694	O	1.761930	-1.525193	-1.891330
N	2.879675	-1.836059	-0.527837	N	0.089823	-2.847402	-1.072266
H	2.600495	-2.294930	-1.388723	H	-0.336291	-2.818750	-1.992803
C	1.440652	3.070550	-0.155947	C	3.605184	0.717460	-0.280101
H	1.379893	4.001856	0.424984	H	4.315275	1.274817	0.346009
C	3.561990	-0.614187	1.742442	C	1.206758	-2.868450	1.349026
H	3.810643	-0.037651	2.626585	H	1.723040	-2.817597	2.301271
O	-3.367364	-3.479414	0.810170	C	0.287291	3.945944	0.400050
C	-3.247124	2.642054	0.509380	H	1.047497	4.433615	1.019594
H	-2.995190	3.390415	1.268424	C	-0.433040	2.918300	1.274352
C	-3.222759	1.270441	1.185195	C	-1.252021	1.951453	0.695222
C	-3.041058	0.108318	0.440213	C	-0.264764	2.933927	2.670905
C	-3.448460	1.172187	2.571129	C	-1.933983	0.996397	1.489107
C	-3.031180	-1.165780	1.060305	H	-1.346945	1.907922	-0.385158
H	-2.907008	0.174792	-0.634639	C	-0.915324	1.986039	3.467779
C	-3.495331	-0.081153	3.189391	H	0.378696	3.680540	3.128082
H	-3.594020	2.074809	3.158337	C	-1.735913	1.022407	2.896397
C	-3.292161	-1.242424	2.454617	H	-0.780349	2.005520	4.545785
H	-3.674406	-0.147233	4.259044	H	-2.252554	0.300067	3.519431
H	-3.292903	-2.210579	2.943778	C	3.047645	-1.394096	0.615736
C	-2.831584	-2.377291	0.295403	H	3.296528	-1.665425	1.644781
C	-2.109356	-2.562064	-0.946079	C	-0.601889	-3.561197	-0.085842
C	-2.419381	-3.667617	-1.784647	O	-1.659101	-4.128095	-0.357774
C	-1.033762	-1.715442	-1.319900	C	0.041102	-3.545311	1.220728
C	-1.710357	-3.882661	-2.960799	C	-0.630965	-4.261150	2.357278
H	-3.237890	-4.325141	-1.511176	H	-0.045303	-4.177836	3.276986
C	-0.347086	-1.932524	-2.506818	H	-1.627047	-3.842211	2.540896
H	-0.737840	-0.900126	-0.668169	H	-0.766739	-5.324366	2.128094

C	-0.676707	-3.017106	-3.336011	C	1.023678	3.208842	-0.714678
H	-1.971421	-4.724908	-3.595804	O	0.650835	3.131451	-1.869642
H	0.465447	-1.262689	-2.774906	O	-2.875393	-1.156611	1.617299
H	-0.128726	-3.185280	-4.258398	C	-2.738724	-0.047621	0.896125
C	3.004504	1.609246	0.818426	C	-3.431088	-0.059584	-0.377180
H	3.367374	1.804917	1.830950	C	-3.708473	-1.298741	-1.017344
C	3.314235	-2.672266	0.510338	C	-3.914556	1.133117	-0.974222
O	3.360038	-3.888557	0.347078	C	-4.406299	-1.327336	-2.219880
C	3.676926	-1.962824	1.730619	H	-3.333372	-2.218877	-0.581728
C	4.149357	-2.763143	2.910754	C	-4.592767	1.086711	-2.184203
H	4.378874	-2.114124	3.760358	H	-3.760324	2.084628	-0.476231
H	3.387661	-3.486638	3.223730	C	-4.848401	-0.141244	-2.815632
H	5.049505	-3.336753	2.660706	H	-4.596536	-2.281598	-2.703765
C	-2.166854	2.712522	-0.563768	H	-4.941209	2.011302	-2.636383
O	-2.354914	2.571874	-1.757287	H	-5.388277	-0.168087	-3.757515

CI^{T_1/T_2}_2

O	1.724706	2.653145	0.620211
C	3.052022	2.384522	0.116719
H	2.983570	2.052828	-0.923882
H	3.644618	3.303566	0.156882
O	2.896275	0.108404	0.944448
C	5.117914	0.951753	0.541531
C	4.900934	-0.380233	-0.190397
H	5.531603	1.713312	-0.124247
H	5.791017	-1.013097	-0.170701
H	4.617648	-0.197783	-1.232444
O	6.037323	0.874759	1.623000
H	5.721109	0.212983	2.261179
N	2.905232	-1.928898	-0.223476
C	3.072500	-3.292908	0.017524
O	3.840340	-3.732253	0.868741
N	2.311274	-4.119716	-0.782759
H	2.431913	-5.113226	-0.619683
C	3.679479	1.319267	0.997319
H	3.702699	1.669985	2.035596
C	2.054698	-1.451290	-1.207233
H	1.962063	-0.377739	-1.271139
O	-3.210143	0.050705	2.727842
C	-4.989457	-0.511052	1.295741
C	-5.883685	-0.044098	0.305410
C	-5.388951	-1.595658	2.114654
C	-7.110148	-0.672474	0.112109
H	-5.622571	0.819516	-0.296790
C	-6.615843	-2.218535	1.913179
H	-4.711399	-1.948344	2.884858
C	-7.481743	-1.764802	0.909508
H	-7.785057	-0.306097	-0.656386
H	-6.899958	-3.062665	2.535312
H	-8.439990	-2.251719	0.753439

$^3RC^*_2$

O	1.865226	2.369580	0.353807
C	3.133857	2.147802	-0.299838
H	2.972263	1.506619	-1.172225
H	3.541145	3.104450	-0.638083
O	3.529596	0.271836	1.237038
C	5.444239	1.143012	0.125443
C	5.220712	-0.308207	-0.325733
H	5.716660	1.792218	-0.710179
H	6.147996	-0.883080	-0.342706
H	4.777115	-0.334428	-1.326260
O	6.497684	1.291191	1.069328
H	6.282413	0.770879	1.861110
N	3.233617	-1.800690	0.125906
C	3.682976	-3.114895	-0.000674
O	4.804334	-3.457127	0.362351
N	2.791458	-4.003816	-0.568619
H	3.103179	-4.966585	-0.608723
C	4.067376	1.508777	0.717719
H	4.182873	2.185780	1.569526
C	2.031437	-1.343802	-0.410390
H	1.685508	-0.402558	-0.003588
O	-2.911205	-1.028372	1.468999
C	-5.084816	-0.741513	0.580929
C	-6.070028	0.194328	0.224679
C	-5.470434	-2.056963	0.892786
C	-7.412611	-0.182824	0.174188
H	-5.792757	1.221215	0.011178
C	-6.807690	-2.435623	0.824465
H	-4.705331	-2.770390	1.181216
C	-7.782216	-1.497623	0.465550
H	-8.168736	0.550531	-0.090660
H	-7.094151	-3.458217	1.052999
H	-8.827090	-1.791426	0.417533

C	3.716416	-0.992964	0.565073	C	4.212637	-0.850320	0.704731
H	4.042009	-1.551947	1.445353	H	4.704796	-1.392853	1.514184
C	1.426840	-3.751201	-1.817255	C	1.425602	-3.762590	-0.845972
O	0.837153	-4.637015	-2.454085	O	0.697477	-4.712769	-1.176938
C	1.302204	-2.333560	-2.025724	C	1.021580	-2.397253	-0.742185
C	0.395878	-1.797677	-3.086811	C	-0.385249	-1.992647	-0.957706
H	-0.320358	-1.079517	-2.665558	H	-0.824174	-1.583017	-0.033445
H	0.966585	-1.260447	-3.857301	H	-0.442996	-1.182697	-1.700313
H	-0.154490	-2.610296	-3.564611	H	-0.990357	-2.838341	-1.288801
C	-3.693473	0.135273	1.557464	C	-3.640039	-0.380739	0.715577
C	-2.928068	0.880476	0.544577	C	-3.064553	0.764482	-0.060030
C	-2.027956	1.883800	0.976517	C	-2.015108	1.493126	0.523480
C	-3.009376	0.589557	-0.835188	C	-3.471228	1.073479	-1.365975
C	-1.275408	2.622043	0.065665	C	-1.389648	2.536019	-0.160052
H	-1.954568	2.094978	2.038557	H	-1.701050	1.234873	1.530451
C	-2.251558	1.320082	-1.745718	C	-2.826940	2.092295	-2.070115
H	-3.648796	-0.212754	-1.186551	H	-4.263154	0.504205	-1.841448
C	-1.394057	2.336598	-1.306306	C	-1.800469	2.822346	-1.472551
H	-2.322931	1.096960	-2.806461	H	-3.126497	2.316785	-3.089688
H	-0.811604	2.900289	-2.029569	H	-1.304404	3.610665	-2.030205
C	1.021704	3.595250	-0.036332	C	1.011908	3.217940	-0.255804
O	1.457702	4.211200	-0.991331	O	1.263217	3.791033	-1.297853
C	-0.375477	3.755684	0.554566	C	-0.292923	3.350051	0.523586
H	-0.275807	3.656396	1.640313	H	-0.124474	2.923289	1.515761
C	-0.957716	5.139010	0.220690	C	-0.671049	4.836727	0.669978
H	-1.054761	5.273629	-0.860447	H	-0.795804	5.308320	-0.308654
H	-1.948242	5.241973	0.674127	H	-1.609882	4.928461	1.224145
H	-0.313205	5.934543	0.609010	H	0.106814	5.381571	1.215497

$^{3}TS_{1}^{*}$(a)

C	4.107671	-3.266710	0.520341
H	4.255189	-4.052626	-0.226727
H	5.021760	-3.180742	1.117165
H	3.295307	-3.571352	1.186303
O	3.646119	0.395091	0.219855
C	3.104715	1.543322	0.911668
H	2.547025	1.212270	1.789664
H	3.932636	2.184702	1.227420
O	1.099726	1.476394	-0.416676
C	1.592732	3.589801	0.458680
C	0.384379	3.755548	-0.490588
H	1.243899	3.440770	1.487241
H	0.686741	4.385288	-1.332389
H	-0.480638	4.207384	-0.007610
O	2.552174	4.631097	0.387034
H	2.216828	5.382822	0.900185
N	-1.212792	1.737059	-0.737071
C	-1.796032	1.841285	0.541170
O	-1.263532	2.418488	1.472829

$^{3}IM_{1}^{*}$

C	-3.591198	-3.725939	-0.251496
H	-3.643177	-4.452277	0.565347
H	-4.490645	-3.832526	-0.866798
H	-2.724673	-3.967060	-0.873683
O	-3.701617	-0.027302	-0.300750
C	-3.299456	1.125143	-1.077064
H	-2.687612	0.800028	-1.920385
H	-4.198524	1.624353	-1.449260
O	-1.340583	1.409129	0.282414
C	-2.042737	3.361635	-0.798590
C	-0.877505	3.749942	0.137210
H	-1.660104	3.154572	-1.805014
H	-1.262686	4.418645	0.912988
H	-0.060956	4.248255	-0.383127
O	-3.114266	4.291210	-0.837955
H	-2.850129	5.026764	-1.412404
N	0.925689	1.949652	0.581240
C	1.498238	2.002257	-0.677754
O	0.938552	2.431183	-1.679066

N	-3.045291	1.256766	0.640698	N	2.820090	1.551497	-0.731859
H	-3.490220	1.356948	1.547758	H	3.269293	1.683856	-1.632765
C	2.223781	2.293050	-0.066246	C	-2.536337	2.057272	-0.157554
H	2.809086	2.531948	-0.968000	H	-3.169837	2.312253	0.707115
C	-1.808641	1.012526	-1.726303	C	1.584963	1.374769	1.658701
H	-1.276238	0.984488	-2.668549	H	1.082538	1.445006	2.612669
O	-2.313554	-1.638713	-1.313053	O	2.463225	-0.934791	1.477715
C	3.781915	-1.939882	-0.177636	C	-3.485083	-2.306199	0.319708
H	4.615398	-1.653927	-0.828836	H	-4.368609	-2.087917	0.929353
C	2.514033	-1.992680	-1.035421	C	-2.246731	-2.086006	1.193453
C	1.269407	-2.015852	-0.410659	C	-0.992642	-2.009561	0.589857
C	2.584203	-1.947973	-2.435836	C	-2.360489	-1.879386	2.574585
C	0.058282	-1.858890	-1.138339	C	0.160738	-1.600028	1.306685
H	1.235211	-2.103402	0.667539	H	-0.918350	-2.210326	-0.470580
C	1.397541	-1.917066	-3.186174	C	-1.214636	-1.586666	3.327292
H	3.549801	-1.932022	-2.934346	H	-3.332316	-1.940329	3.057141
C	0.161929	-1.857066	-2.561841	C	0.018949	-1.428187	2.713000
H	1.450764	-1.908584	-4.272166	H	-1.297451	-1.454401	4.402933
H	-0.748117	-1.787960	-3.146565	H	0.890123	-1.169876	3.302902
C	-1.227945	-1.680230	-0.515004	C	1.416837	-1.335556	0.661060
C	-1.483560	-1.643907	0.929217	C	1.766432	-1.589413	-0.740748
C	-2.703276	-2.195686	1.398978	C	3.038781	-2.135202	-1.032098
C	-0.623668	-1.058048	1.890188	C	0.914127	-1.290960	-1.828321
C	-3.018662	-2.205622	2.752745	C	3.420903	-2.407206	-2.341918
H	-3.387050	-2.624507	0.675051	H	3.716808	-2.349347	-0.213086
C	-0.951685	-1.060050	3.244031	C	1.306530	-1.558877	-3.138708
H	0.273726	-0.543153	1.568712	H	-0.034609	-0.796851	-1.652994
C	-2.142944	-1.642127	3.688995	C	2.555109	-2.126797	-3.404339
H	-3.952289	-2.654132	3.083009	H	4.398054	-2.841529	-2.535807
H	-0.278518	-0.588355	3.955290	H	0.637102	-1.307452	-3.956899
H	-2.392172	-1.644426	4.746446	H	2.855573	-2.336943	-4.426919
C	0.118378	2.320948	-1.003374	C	-0.456135	2.409963	0.785733
H	0.211515	2.289441	-2.092959	H	-0.563733	2.473089	1.872618
C	-3.752404	0.528290	-0.317666	C	3.553963	0.876492	0.225109
O	-4.884918	0.130086	-0.092514	O	4.719111	0.571761	0.032523
C	-3.018894	0.321458	-1.584968	C	2.793425	0.530154	1.513538
C	-3.812574	-0.081369	-2.791183	C	3.720168	0.645638	2.721343
H	-3.151920	-0.366072	-3.612775	H	3.175338	0.382974	3.632294
H	-4.464067	-0.920788	-2.544540	H	4.565531	-0.034277	2.598389
H	-4.441558	0.754782	-3.122766	H	4.098332	1.667344	2.817441
C	3.580273	-0.808725	0.829852	C	-3.420193	-1.254734	-0.787796
O	3.325329	-0.957648	2.009187	O	-3.089657	-1.471108	-1.937687

ISC^{T_1/S_0}_1

C	4.280328	-2.978652	0.873825
H	4.480091	-3.844497	0.235094
H	5.189455	-2.747919	1.438370
H	3.496172	-3.248690	1.586840
O	3.564183	0.574605	0.108110

$^1Oxe_1$

C	4.529404	-2.588499	0.811351
H	4.715261	-3.484833	0.211982
H	5.461318	-2.305874	1.311167
H	3.789489	-2.832979	1.579131
O	3.570414	0.877598	-0.106288

C	3.011392	1.779638	0.689508	C	3.063530	2.098337	0.476796
H	2.498264	1.532585	1.620589	H	2.756058	1.909290	1.506850
H	3.829496	2.474308	0.901187	H	3.868645	2.839505	0.469450
O	0.973022	1.505108	-0.553428	O	0.841512	1.623634	-0.333991
C	1.393144	3.705445	0.077899	C	1.290439	3.931158	0.102172
C	0.177713	3.737244	-0.877454	C	-0.182030	3.568415	0.392950
H	1.051353	3.632229	1.118804	H	1.786070	4.312441	1.004122
H	0.470705	4.272381	-1.785963	H	-0.859573	4.397035	0.182840
H	-0.693139	4.220778	-0.443254	H	-0.304406	3.269660	1.435166
O	2.308794	4.774900	-0.085423	O	1.440754	4.855549	-0.972996
H	1.925338	5.564320	0.327564	H	1.134639	5.721843	-0.659241
N	-1.341107	1.608648	-0.918369	N	-1.477326	1.425068	-0.303050
C	-2.126035	1.973628	0.163731	C	-2.605223	1.760918	0.405353
O	-1.878637	2.884204	0.944120	O	-2.744872	2.758130	1.099054
N	-3.304130	1.226976	0.298068	N	-3.682348	0.857437	0.299980
H	-3.903363	1.541710	1.055279	H	-4.463667	1.094483	0.903433
C	2.071722	2.390701	-0.330028	C	1.905753	2.587752	-0.373493
H	2.620630	2.559737	-1.270144	H	2.238855	2.719543	-1.411605
C	-1.555021	0.416812	-1.592401	C	-1.405670	0.207302	-1.087213
H	-0.888724	0.231608	-2.423248	H	-0.767727	0.400647	-1.949781
O	-2.287248	-1.777974	-1.098103	O	-2.145101	-1.779643	-1.228936
C	3.850029	-1.782978	0.012381	C	4.024066	-1.452426	-0.091214
H	4.648370	-1.537068	-0.697073	H	4.790424	-1.221335	-0.841439
C	2.578338	-2.057301	-0.795222	C	2.742869	-1.823725	-0.839303
C	1.335476	-1.940412	-0.178014	C	1.493642	-1.508078	-0.298513
C	2.639033	-2.384938	-2.157023	C	2.796658	-2.480082	-2.074849
C	0.124488	-2.012820	-0.910262	C	0.306622	-1.758733	-0.993904
H	1.300170	-1.722384	0.881508	H	1.447459	-1.020542	0.667180
C	1.451945	-2.581448	-2.875975	C	1.616540	-2.793786	-2.750322
H	3.601406	-2.481390	-2.652948	H	3.758668	-2.738178	-2.511135
C	0.213233	-2.384516	-2.279351	C	0.376597	-2.419315	-2.227137
H	1.502093	-2.860074	-3.925327	H	1.662199	-3.311729	-3.704564
H	-0.697003	-2.497450	-2.857810	H	-0.535196	-2.633128	-2.772981
C	-1.129720	-1.638690	-0.314556	C	-1.019109	-1.211321	-0.478755
C	-1.369672	-1.419917	1.119153	C	-1.227418	-1.403341	1.019171
C	-2.459460	-2.076990	1.733834	C	-1.996386	-2.488651	1.463586
C	-0.578761	-0.561552	1.914411	C	-0.647476	-0.550832	1.971438
C	-2.719242	-1.914315	3.091362	C	-2.179487	-2.719991	2.827283
H	-3.090934	-2.721920	1.132492	H	-2.459047	-3.143526	0.733224
C	-0.848537	-0.399083	3.272617	C	-0.835366	-0.782909	3.336477
H	0.210638	0.019468	1.451350	H	-0.054592	0.298522	1.650402
C	-1.911612	-1.080129	3.871014	C	-1.600135	-1.867077	3.769710
H	-3.553575	-2.442929	3.544578	H	-2.778194	-3.566586	3.152539
H	-0.230974	0.272830	3.862519	H	-0.383060	-0.110044	4.059984
H	-2.117099	-0.953539	4.930083	H	-1.745755	-2.044598	4.831714
C	-0.051052	2.248420	-1.225809	C	-0.373374	2.359205	-0.521660
H	0.063727	2.107266	-2.305439	H	-0.420248	2.690005	-1.571901
C	-3.715676	0.084095	-0.360718	C	-3.870842	-0.203315	-0.558435
O	-4.775173	-0.456128	-0.090307	O	-4.896534	-0.863675	-0.554882
C	-2.772401	-0.441013	-1.457165	C	-2.711317	-0.473562	-1.519686

C	-3.566043	-0.619612	-2.755227	C	-3.171510	-0.346164	-2.960558
H	-2.906580	-0.999913	-3.540217	H	-2.351334	-0.599082	-3.638233
H	-4.380705	-1.329627	-2.589368	H	-4.011903	-1.022317	-3.142486
H	-3.990710	0.334618	-3.081824	H	-3.499493	0.678249	-3.169520
C	3.604556	-0.540308	0.869049	C	3.793015	-0.173980	0.712196
O	3.409129	-0.548923	2.068903	O	3.766338	-0.106320	1.924859

$^{3}TS^{*}_{1}$ (b)

C	4.190300	-3.024863	0.833382
H	4.297713	-3.914189	0.204768
H	5.154953	-2.821459	1.310993
H	3.458539	-3.239610	1.616816
O	3.680882	0.539889	0.069240
C	3.159733	1.785835	0.588742
H	2.692388	1.608787	1.558857
H	3.994013	2.482639	0.704924
O	1.092328	1.395101	-0.554905
C	1.466984	3.639091	-0.076459
C	0.227949	3.578122	-0.998013
H	1.153652	3.616451	0.976101
H	0.493028	4.036637	-1.955586
H	-0.637128	4.089265	-0.584088
O	2.342615	4.724717	-0.327255
H	1.939354	5.525742	0.042556
N	-1.246209	1.432782	-0.795551
C	-2.070334	1.940870	0.193095
O	-1.821895	2.908039	0.900091
N	-3.303380	1.282231	0.319212
H	-3.903105	1.675002	1.038262
C	2.171053	2.322675	-0.427462
H	2.682189	2.446861	-1.395641
C	-1.461956	0.131302	-1.305638
H	-0.886418	-0.021185	-2.214333
O	-2.449934	-1.784806	-0.966072
C	3.739650	-1.830769	-0.020366
H	4.505525	-1.607896	-0.770459
C	2.419785	-2.078300	-0.756506
C	1.235253	-2.075873	-0.089850
C	2.434377	-2.309279	-2.191586
C	-0.051015	-2.149358	-0.806944
H	1.220824	-1.932411	0.984498
C	1.213286	-2.622306	-2.874580
H	3.379114	-2.326621	-2.724892
C	0.015352	-2.593639	-2.229191
H	1.260127	-2.912107	-3.921718
H	-0.905818	-2.861361	-2.734779
C	-1.189573	-1.415150	-0.342129
C	-1.342466	-1.197312	1.148807
C	-2.324500	-1.924720	1.840455

$^{3}Oxe^{*}_{1}$

C	4.852172	-2.223535	-0.440114
H	4.929594	-3.056075	-1.145785
H	5.797846	-1.672355	-0.461917
H	4.721991	-2.627483	0.567936
O	3.429828	1.030226	-0.401821
C	2.927901	2.145092	0.372198
H	2.557671	1.780851	1.332249
H	3.743864	2.852804	0.542120
O	0.872408	1.769430	-0.769506
C	0.993525	3.874315	0.228419
C	-0.304053	3.832380	-0.605229
H	0.779979	3.580657	1.264597
H	-0.159198	4.464497	-1.487334
H	-1.177979	4.179152	-0.059021
O	1.695184	5.104940	0.176445
H	1.229785	5.737520	0.745878
N	-1.451895	1.498100	-0.541022
C	-2.148744	1.757877	0.615467
O	-1.874216	2.618925	1.439695
N	-3.304682	0.975192	0.801686
H	-3.811872	1.194352	1.653511
C	1.827142	2.784585	-0.455888
H	2.257905	3.199091	-1.380439
C	-1.635605	0.238390	-1.230654
H	-1.245824	0.346356	-2.243846
O	-2.499314	-1.698107	-1.048580
C	3.692943	-1.294014	-0.820970
H	3.911504	-0.825552	-1.785594
C	2.314022	-1.972639	-0.936054
C	1.266277	-1.293085	-1.498752
C	2.112991	-3.337122	-0.530058
C	-0.099116	-1.885719	-1.449520
H	1.405650	-0.297664	-1.908095
C	0.902710	-4.034507	-0.885766
H	2.925015	-3.898524	-0.084355
C	-0.153431	-3.373574	-1.427674
H	0.877648	-5.116467	-0.771955
H	-1.043388	-3.892187	-1.771154
C	-1.183519	-1.168610	-0.652933
C	-0.973666	-1.309562	0.848453
C	-1.699976	-2.276296	1.561782

C	-0.521576	-0.315547	1.867164	C	-0.003891	-0.553506	1.524075
C	-2.474854	-1.780535	3.219517	C	-1.465911	-2.476391	2.922665
H	-2.970405	-2.598779	1.288243	H	-2.456851	-2.857583	1.046923
C	-0.677693	-0.170594	3.248318	C	0.225124	-0.755258	2.886481
H	0.228460	0.267439	1.344061	H	0.561562	0.197747	0.986413
C	-1.652081	-0.901752	3.929367	C	-0.502203	-1.717018	3.591114
H	-3.236019	-2.355894	3.739769	H	-2.039518	-3.226310	3.461237
H	-0.036134	0.519905	3.789149	H	0.979401	-0.160074	3.393859
H	-1.772391	-0.786258	5.003062	H	-0.321294	-1.872317	4.651305
C	0.009416	2.062880	-1.217423	C	-0.398370	2.364450	-1.070666
H	0.074803	1.838522	-2.287786	H	-0.535996	2.328532	-2.156742
C	-3.793416	0.169024	-0.339595	C	-3.866002	0.014870	-0.015383
O	-4.904574	-0.274412	-0.099426	O	-4.931357	-0.513846	0.256155
C	-2.857259	-0.451573	-1.384748	C	-3.046448	-0.367486	-1.256050
C	-3.542511	-0.502450	-2.742540	C	-3.878699	-0.270075	-2.518783
H	-2.883878	-0.977504	-3.474818	H	-3.299564	-0.632525	-3.372767
H	-4.469807	-1.077851	-2.665768	H	-4.784811	-0.873838	-2.415006
H	-3.788289	0.507185	-3.088537	H	-4.173632	0.768766	-2.704168
C	3.547689	-0.573612	0.824185	C	3.557576	-0.169162	0.206501
O	3.257112	-0.565951	2.004664	O	3.531224	-0.329169	1.410303

^{1}Oxe$^{*}_{1}$

C	4.466178	-2.641266	0.750682
H	4.650216	-3.515519	0.118973
H	5.388995	-2.400974	1.288177
H	3.699468	-2.901381	1.486358
O	3.610860	0.878681	-0.051720
C	3.097461	2.086269	0.552889
H	2.806234	1.882363	1.584766
H	3.895980	2.834149	0.540613
O	0.857721	1.613372	-0.211119
C	1.321505	3.923439	0.193856
C	-0.156460	3.577166	0.475908
H	1.815394	4.298364	1.099495
H	-0.825580	4.407939	0.246884
H	-0.291435	3.295345	1.520747
O	1.492691	4.846448	-0.879510
H	1.199053	5.717153	-0.566141
N	-1.468768	1.440532	-0.206697
C	-2.591229	1.789946	0.523467
O	-2.674053	2.765490	1.273888
N	-3.694972	0.978566	0.354558
H	-4.474941	1.232453	0.948975
C	1.924056	2.572222	-0.277347
H	2.239878	2.695265	-1.322332
C	-1.437373	0.258975	-1.038444
H	-0.842020	0.483372	-1.926007
O	-2.133036	-1.716161	-1.339265
C	4.012047	-1.457215	-0.116171

CI$^{S_1/S_2}_{1}$

C	4.319130	-2.815238	0.839570
H	4.471764	-3.704867	0.220899
H	5.246403	-2.607330	1.383357
H	3.533670	-3.031886	1.569882
O	3.659356	0.732647	-0.018001
C	3.200539	1.979183	0.558202
H	2.923038	1.819673	1.601421
H	4.025953	2.694601	0.502351
O	0.928707	1.567999	-0.131978
C	1.484058	3.874180	0.134804
C	-0.033440	3.630279	0.317809
H	1.931566	4.229911	1.071672
H	-0.628394	4.469069	-0.052471
H	-0.271086	3.463401	1.367054
O	1.804729	4.763578	-0.931137
H	1.560036	5.660232	-0.648088
N	-1.411317	1.504944	-0.285844
C	-2.420531	1.751812	0.626463
O	-2.384072	2.589869	1.536438
N	-3.547089	0.975615	0.454039
H	-4.292422	1.171075	1.111996
C	2.028445	2.475003	-0.266418
H	2.325614	2.533400	-1.323500
C	-1.432852	0.309129	-1.104398
H	-0.794633	0.480636	-1.973070
O	-2.231542	-1.657802	-1.257617
C	3.925833	-1.625450	-0.049517

H	4.803022	-1.212863	-0.835740	H	4.733219	-1.428189	-0.765113
C	2.742364	-1.763406	-0.911287	C	2.651605	-1.893531	-0.852537
C	1.486860	-1.492249	-0.360471	C	1.401459	-1.562628	-0.320105
C	2.811813	-2.311172	-2.197671	C	2.711170	-2.466733	-2.128511
C	0.308921	-1.685234	-1.088533	C	0.223532	-1.718748	-1.058371
H	1.429142	-1.085628	0.641694	H	1.351741	-1.133928	0.673276
C	1.640380	-2.563603	-2.912878	C	1.536288	-2.685952	-2.851250
H	3.779368	-2.532707	-2.641568	H	3.673649	-2.733739	-2.558304
C	0.394021	-2.236422	-2.374178	C	0.298165	-2.299110	-2.331309
H	1.697762	-2.997265	-3.907590	H	1.586114	-3.139772	-3.837500
H	-0.509875	-2.405518	-2.948159	H	-0.606808	-2.441590	-2.912532
C	-1.023993	-1.191922	-0.536393	C	-1.085661	-1.145316	-0.539375
C	-1.232679	-1.508315	0.938959	C	-1.309742	-1.380270	0.952417
C	-1.939479	-2.666742	1.294908	C	-2.089105	-2.494646	1.336926
C	-0.692268	-0.705414	1.954671	C	-0.753549	-0.562536	1.949303
C	-2.104859	-3.014599	2.634886	C	-2.308815	-2.779852	2.683575
H	-2.367783	-3.286911	0.514674	H	-2.511156	-3.131510	0.567889
C	-0.864187	-1.054285	3.297539	C	-0.968032	-0.857916	3.294928
H	-0.139960	0.192720	1.701230	H	-0.143559	0.291142	1.677994
C	-1.569210	-2.207529	3.642840	C	-1.752951	-1.961417	3.668553
H	-2.656530	-3.914846	2.892097	H	-2.910350	-3.640336	2.961516
H	-0.444620	-0.418223	4.072254	H	-0.520837	-0.228965	4.059250
H	-1.702090	-2.475806	4.687323	H	-1.920356	-2.176776	4.719797
C	-0.352398	2.354835	-0.420466	C	-0.237196	2.337913	-0.475612
H	-0.380238	2.672342	-1.476392	H	-0.180857	2.562503	-1.552445
C	-3.810995	-0.214512	-0.379653	C	-3.888783	0.217656	-0.684925
O	-5.035431	-0.612093	-0.634216	O	-5.108540	-0.214192	-0.776275
C	-2.758203	-0.415704	-1.477295	C	-2.790997	-0.238623	-1.559144
C	-3.291486	-0.190993	-2.882866	C	-3.179945	-0.230551	-3.032462
H	-2.490489	-0.320114	-3.616935	H	-2.387037	-0.663468	-3.648260
H	-4.091585	-0.902698	-3.103597	H	-4.098038	-0.811317	-3.166979
H	-3.696983	0.821951	-2.973768	H	-3.366303	0.797339	-3.361123
C	3.782703	-0.207818	0.732152	C	3.745567	-0.353440	0.778073
O	3.715605	-0.188658	1.944984	O	3.651546	-0.316630	1.990224

$^{1}IM_{1}^{*}$

C	-4.330171	-2.928519	-1.017425
H	-4.661630	-3.718542	-0.336368
H	-5.124705	-2.747277	-1.749208
H	-3.448576	-3.286193	-1.556978
O	-3.611443	0.666195	-0.485769
C	-2.892559	1.787478	-1.041821
H	-2.297735	1.459757	-1.896197
H	-3.621167	2.535734	-1.367561
O	-0.951672	1.474765	0.361075
C	-1.337586	3.704323	-0.288611
C	-0.138123	3.697017	0.687964
H	-0.982576	3.688451	-1.324248
H	-0.421513	4.235104	1.596562

$ISC_{1}^{S_1/T_1}$

C	0.766506	4.839190	-0.141317
H	0.407342	5.431534	0.705992
H	1.452750	5.459280	-0.728759
H	-0.088089	4.589634	-0.775649
O	3.042663	1.979298	-0.408844
C	3.402072	0.842118	-1.217641
H	2.591191	0.617516	-1.912688
H	4.311420	1.074246	-1.780661
O	2.455907	-0.558317	0.482674
C	4.017648	-1.645209	-0.964913
C	3.346135	-2.703532	-0.054661
H	3.590182	-1.682739	-1.970344
H	4.095257	-3.084046	0.644746

H	0.757630	4.162862	0.276459	H	2.931024	-3.549564	-0.604286
O	-2.258452	4.760082	-0.077466	O	5.430982	-1.747329	-1.015092
H	-1.917612	5.550494	-0.524442	H	5.659737	-2.417357	-1.677999
N	1.381858	1.628528	0.650772	N	0.849101	-2.251761	0.438867
C	1.853723	1.780692	-0.694645	C	0.396145	-2.214065	-0.932306
O	1.196480	2.343226	-1.542119	O	1.154036	-1.946696	-1.833181
N	3.105810	1.259146	-0.915717	N	-0.929614	-2.521912	-1.104493
H	3.446128	1.343021	-1.869216	H	-1.257542	-2.510281	-2.066845
C	-2.028183	2.377617	0.052912	C	3.659907	-0.317556	-0.275021
H	-2.644124	2.532467	0.951170	H	4.463297	-0.062469	0.427664
C	2.100668	0.979678	1.576420	C	0.008240	-2.447528	1.447448
H	1.647248	0.878384	2.553673	H	0.423782	-2.407112	2.446779
O	1.815822	-1.919038	1.825612	O	-3.443273	0.086126	1.882430
C	-4.013379	-1.656551	-0.221117	C	1.472468	3.575555	0.368132
H	-4.915999	-1.316245	0.298926	H	2.349076	3.861888	0.958187
C	-2.907523	-1.834807	0.824022	C	0.591336	2.673724	1.242636
C	-1.591046	-1.994620	0.392736	C	-0.595788	2.150757	0.729121
C	-3.188090	-1.745313	2.195120	C	1.005325	2.331713	2.541392
C	-0.494512	-1.951402	1.290466	C	-1.416638	1.253961	1.466912
H	-1.410341	-2.106144	-0.668472	H	-0.904472	2.462968	-0.260485
C	-2.127639	-1.807293	3.111983	C	0.200897	1.475690	3.305662
H	-4.211027	-1.616909	2.539101	H	1.932644	2.729746	2.944250
C	-0.812359	-1.888439	2.678221	C	-0.975258	0.948497	2.788961
H	-2.338064	-1.758212	4.178464	H	0.502894	1.220322	4.319682
H	0.006819	-1.885606	3.388730	H	-1.610089	0.310985	3.393313
C	0.908278	-1.920827	0.895836	C	-2.688650	0.675021	1.021595
C	1.377149	-1.923674	-0.505464	C	-3.153085	0.745425	-0.386012
C	2.623876	-2.546947	-0.775160	C	-4.545129	0.615088	-0.621923
C	0.727165	-1.298506	-1.599275	C	-2.328668	0.833926	-1.536297
C	3.160338	-2.584350	-2.057000	C	-5.080085	0.615455	-1.905008
H	3.149335	-3.013745	0.051465	H	-5.189503	0.510152	0.244861
C	1.275242	-1.330934	-2.881556	C	-2.865767	0.820829	-2.824413
H	-0.185253	-0.736624	-1.440203	H	-1.249956	0.872984	-1.431588
C	2.489186	-1.979695	-3.128482	C	-4.245421	0.722642	-3.026748
H	4.108764	-3.089429	-2.226246	H	-6.156530	0.526200	-2.038041
H	0.753045	-0.828945	-3.692947	H	-2.194501	0.875065	-3.679329
H	2.908305	-2.007094	-4.130468	H	-4.660571	0.717619	-4.031055
C	0.053981	2.201147	1.027551	C	2.295094	-1.917969	0.745373
H	-0.005906	2.032872	2.106351	H	2.370671	-2.119691	1.816277
C	3.935859	0.596361	-0.012178	C	-1.877864	-2.790593	-0.122368
O	5.038368	0.188718	-0.339174	O	-3.030806	-3.064886	-0.391964
C	3.373317	0.456262	1.340669	C	-1.364672	-2.709539	1.264376
C	4.209204	-0.115273	2.423457	C	-2.305521	-2.831109	2.382332
H	3.590637	-0.495050	3.236514	H	-2.828101	-1.851144	2.440219
H	4.844271	-0.910876	2.028924	H	-3.070983	-3.581172	2.163821
H	4.875351	0.665976	2.818018	H	-1.805898	-3.033208	3.330439
C	-3.559098	-0.520421	-1.134945	C	1.964744	2.708445	-0.783803
O	-3.144264	-0.651444	-2.270315	O	1.439835	2.620395	-1.877045

$^{3}TS_{2}^{*}$(a) ----------

$^3IM_2^*$				----------			
O	-3.313485	-0.476488	0.298604	O	-3.531594	0.177197	0.343592
C	-3.421718	0.516382	-0.741514	C	-3.459590	1.209442	-0.658069
H	-2.608800	0.341094	-1.454841	H	-2.858955	0.835586	-1.493847
H	-4.374907	0.406471	-1.264730	H	-4.461387	1.445440	-1.028615
O	-2.207764	2.043354	0.763528	O	-1.620470	2.120726	0.674035
C	-3.122416	2.972989	-1.243953	C	-2.440956	3.469969	-1.126984
C	-1.597184	3.170415	-1.209823	C	-0.929920	3.236584	-1.257211
H	-3.458053	2.608140	-2.217853	H	-2.976292	3.289070	-2.068157
H	-1.295441	4.142323	-1.598459	H	-0.398459	4.097095	-1.665585
H	-1.092041	2.384901	-1.781450	H	-0.718358	2.357571	-1.875595
O	-3.862200	4.166291	-1.027087	O	-2.744918	4.766210	-0.616010
H	-3.623090	4.538898	-0.162631	H	-2.459773	5.416541	-1.278497
N	0.094010	2.504661	0.577781	N	0.717936	2.244417	0.435310
C	1.138449	3.380555	0.265415	C	1.850498	2.988465	0.195233
O	0.938347	4.472847	-0.248148	O	1.823061	4.127061	-0.260214
N	2.407481	2.920443	0.572272	N	3.057997	2.376224	0.526165
H	3.161263	3.564524	0.360291	H	3.880334	2.948299	0.368979
C	-3.333919	1.911420	-0.138018	C	-2.834873	2.450462	-0.038359
H	-4.237278	2.126112	0.441046	H	-3.530108	2.910228	0.671530
C	0.311938	1.267056	1.111872	C	0.771228	0.854899	0.797583
H	-0.571058	0.718204	1.389697	H	-0.128287	0.622321	1.364503
O	0.745638	0.013470	-0.815985	O	0.698191	0.070645	-0.456901
C	2.835285	-1.123972	-0.835741	C	2.474047	-1.531225	-0.747532
C	3.665134	-2.081884	-0.216441	C	3.154828	-2.684062	-0.283885
C	3.448148	-0.124124	-1.621948	C	3.211858	-0.597999	-1.517931
C	5.048349	-2.047333	-0.390603	C	4.494847	-2.897010	-0.594349
H	3.231336	-2.835921	0.431792	H	2.640723	-3.391350	0.357687
C	4.827444	-0.097757	-1.800290	C	4.548812	-0.821413	-1.827864
H	2.816901	0.623203	-2.091437	H	2.711383	0.293308	-1.879443
C	5.636968	-1.062167	-1.188156	C	5.200126	-1.973429	-1.372624
H	5.669211	-2.788531	0.105802	H	4.995914	-3.783141	-0.214169
H	5.276176	0.674496	-2.419834	H	5.086729	-0.095468	-2.431780
H	6.714345	-1.041165	-1.326881	H	6.245343	-2.144460	-1.613668
C	-1.280430	2.994421	0.279166	C	-0.562367	2.942190	0.198110
H	-1.380876	3.937848	0.829401	H	-0.522491	3.877287	0.768449
C	2.726749	1.829583	1.402538	C	3.213172	1.274453	1.367261
O	3.887223	1.661225	1.785874	O	4.313331	0.992661	1.844256
C	1.605338	0.986759	1.737951	C	1.988966	0.534020	1.614293
C	1.731529	-0.089849	2.749973	C	1.933730	-0.487208	2.693736
H	1.236655	0.211615	3.687842	H	2.941285	-0.765152	3.009018
H	1.229177	-1.007567	2.420674	H	1.400143	-0.083719	3.569204
H	2.781192	-0.295427	2.966596	H	1.385688	-1.382438	2.380358
C	1.361033	-1.087584	-0.679469	C	1.077169	-1.264432	-0.441045
C	0.556842	-2.298548	-0.375394	C	0.024987	-2.236047	-0.263843
C	-0.730379	-2.081603	0.147839	C	-1.234421	-1.815639	0.231038
C	0.937427	-3.628351	-0.653042	C	0.155209	-3.605246	-0.623134
C	-1.632579	-3.117848	0.397730	C	-2.312316	-2.689533	0.387523
H	-1.030480	-1.059470	0.327027	H	-1.374701	-0.771159	0.472788
C	0.049447	-4.671585	-0.403899	C	-0.911096	-4.477895	-0.460868

H	1.903146	-3.844020	-1.096745	H	1.075695	-3.968400	-1.064051
C	-1.229467	-4.429275	0.114916	C	-2.143380	-4.037115	0.041276
H	0.345355	-5.691774	-0.633312	H	-0.795196	-5.519335	-0.748655
H	-1.900423	-5.264887	0.282959	H	-2.958970	-4.743918	0.145247
C	-3.612525	-1.749607	-0.063889	C	-4.038172	-1.009515	-0.063283
O	-4.200841	-2.032766	-1.086730	O	-4.649832	-1.155176	-1.101647
C	-3.035578	-2.760437	0.925570	C	-3.652942	-2.128526	0.900453
H	-2.914483	-2.245719	1.885464	H	-3.472991	-1.668059	1.878301
C	-3.984074	-3.948906	1.103847	C	-4.783251	-3.153295	1.024716
H	-4.169770	-4.453330	0.151334	H	-5.032928	-3.588355	0.052859
H	-3.566845	-4.673214	1.809618	H	-4.501871	-3.958970	1.709130
H	-4.945873	-3.608505	1.500007	H	-5.683325	-2.673285	1.421352

$ISC_2^{T_1/S_0}$

O	-3.480668	-0.147859	0.113039	O	-3.028138	1.539926	-0.013038
C	-3.443728	0.931606	-0.844920	C	-3.459161	0.471523	0.859554
H	-2.713642	0.679496	-1.620893	H	-2.664198	0.272438	1.584702
H	-4.423920	1.044523	-1.317341	H	-4.349814	0.789208	1.409990
O	-1.930748	2.046416	0.738700	O	-2.695132	-1.161496	-0.823664
C	-2.683136	3.324021	-1.128195	C	-4.048094	-1.979975	0.948103
C	-1.151091	3.223087	-1.131410	C	-2.658297	-2.627064	1.022326
H	-3.118125	3.149361	-2.120852	H	-4.423489	-1.680364	1.935204
H	-0.661087	4.137115	-1.471208	H	-2.693511	-3.686458	1.283837
H	-0.814712	2.389016	-1.757033	H	-2.027484	-2.110783	1.753926
O	-3.140483	4.559920	-0.583696	O	-4.992521	-2.807936	0.274606
H	-2.834117	5.271778	-1.168764	H	-5.124922	-3.602992	0.816158
N	0.403487	2.237614	0.650496	N	-0.648004	-2.278263	-0.509741
C	1.557200	2.979128	0.513208	C	0.082713	-3.429551	-0.393229
O	1.563933	4.146846	0.133355	O	-0.403294	-4.527732	-0.153363
N	2.730981	2.309990	0.848324	N	1.465081	-3.288168	-0.592303
H	3.570279	2.875279	0.788058	H	1.981287	-4.159684	-0.525026
C	-3.073989	2.223977	-0.123824	C	-3.786077	-0.769475	0.036136
H	-3.909982	2.558190	0.498330	H	-4.650993	-0.577483	-0.605548
C	0.468479	0.823132	0.849343	C	-0.009078	-1.013855	-0.622363
H	-0.488152	0.505491	1.253142	H	-0.723822	-0.318747	-1.056826
O	0.636209	0.181685	-0.471913	O	0.509458	-0.481451	0.632025
C	2.629369	-1.101900	-0.874749	C	2.904832	0.053788	0.759945
C	3.594327	-2.032150	-0.421443	C	4.181203	0.134320	0.185536
C	3.020469	-0.169303	-1.864865	C	2.792286	-0.028780	2.154354
C	4.874174	-2.052689	-0.967474	C	5.320016	0.141074	0.992745
H	3.361478	-2.698404	0.401181	H	4.295062	0.159666	-0.892651
C	4.296923	-0.208106	-2.416504	C	3.932442	-0.022629	2.959864
H	2.299901	0.563858	-2.208321	H	1.808462	-0.100890	2.605676
C	5.230320	-1.152338	-1.976609	C	5.200533	0.065813	2.382240
H	5.603089	-2.765149	-0.591649	H	6.302261	0.197995	0.531655
H	4.567080	0.503283	-3.192093	H	3.827202	-0.087510	4.039495
H	6.228299	-1.178221	-2.404838	H	6.088553	0.069689	3.008282
C	-0.872359	2.912531	0.341730	C	-2.122353	-2.390422	-0.394532
H	-0.895849	3.832293	0.935194	H	-2.429295	-3.196020	-1.068283

$^1Oxe_2$

C	2.825387	1.149189	1.640932	C	2.167957	-2.208549	-1.101474
O	3.901625	0.856594	2.173990	O	3.338374	-2.327675	-1.427624
C	1.594506	0.410491	1.757487	C	1.377980	-0.916622	-1.273964
C	1.363603	-0.484014	2.929068	C	1.455162	-0.474574	-2.733447
H	2.318690	-0.850371	3.314496	H	2.494637	-0.332601	-3.040779
H	0.865658	0.059807	3.749376	H	1.016098	-1.244085	-3.378746
H	0.721841	-1.336455	2.680418	H	0.908602	0.457140	-2.891463
C	1.267458	-1.048344	-0.357250	C	1.638748	0.121209	-0.072820
C	0.400068	-2.173812	-0.071865	C	1.271014	1.562304	-0.475078
C	-0.969328	-1.900713	0.164166	C	-0.005890	2.026922	-0.145440
C	0.792267	-3.537483	-0.089780	C	2.113718	2.397781	-1.217055
C	-1.921262	-2.893251	0.386421	C	-0.504570	3.250409	-0.599407
H	-1.296688	-0.874586	0.125410	H	-0.618970	1.381298	0.465506
C	-0.145979	-4.532690	0.150192	C	1.646320	3.641316	-1.649358
H	1.810502	-3.821021	-0.321818	H	3.121120	2.088009	-1.475373
C	-1.494289	-4.228685	0.387057	C	0.344338	4.060423	-1.365722
H	0.168485	-5.572330	0.131951	H	2.299503	4.283629	-2.233613
H	-2.197963	-5.036636	0.553777	H	-0.002966	5.014536	-1.751426
C	-3.727346	-1.379962	-0.392140	C	-2.629072	2.667732	0.622665
O	-4.115014	-1.569851	-1.526203	O	-2.761049	2.830576	1.818697
C	-3.387716	-2.477339	0.617200	C	-1.959570	3.663891	-0.322193
H	-3.454950	-2.027435	1.615087	H	-2.500686	3.611434	-1.276171
C	-4.400830	-3.622899	0.514483	C	-2.085730	5.085816	0.249152
H	-4.349455	-4.109057	-0.464046	H	-1.572559	5.161394	1.211646
H	-4.221154	-4.372588	1.289778	H	-1.651592	5.818320	-0.436029
H	-5.416600	-3.239376	0.651171	H	-3.137832	5.347217	0.399817

^{3}TS$_2^*$ (b)

O	-3.329510	0.796917	-0.062895
C	-3.473433	-0.318741	0.844757
H	-2.652637	-0.278718	1.567934
H	-4.415235	-0.225815	1.393404
O	-2.360625	-1.740015	-0.848445
C	-3.329068	-2.826955	1.029955
C	-1.812633	-3.063727	1.018717
H	-3.709534	-2.595136	2.033450
H	-1.533952	-4.075598	1.318339
H	-1.302013	-2.353489	1.677955
O	-4.048555	-3.913323	0.452366
H	-3.914735	-4.689756	1.020091
N	-0.083621	-2.295866	-0.706719
C	0.937238	-3.209567	-0.540533
O	0.766951	-4.374429	-0.183105
N	2.203468	-2.699616	-0.792499
H	2.955685	-3.374073	-0.714409
C	-3.470753	-1.634019	0.068145
H	-4.387499	-1.722603	-0.522188
C	0.192607	-0.898651	-0.745466
H	-0.691407	-0.404675	-1.140901

^{3}Oxe$_2^*$

O	-3.067742	1.415659	-0.053116
C	-3.475209	0.336693	0.818511
H	-2.689186	0.176043	1.562659
H	-4.388283	0.624491	1.348189
O	-2.633315	-1.294528	-0.842238
C	-3.962378	-2.132453	0.933574
C	-2.543169	-2.706885	1.045375
H	-4.371043	-1.835975	1.908367
H	-2.529423	-3.760997	1.327801
H	-1.953058	-2.146162	1.778145
O	-4.849939	-3.018303	0.257112
H	-4.950776	-3.811443	0.808217
N	-0.525092	-2.269908	-0.458069
C	0.278474	-3.353694	-0.212455
O	-0.130811	-4.460369	0.119297
N	1.653506	-3.080678	-0.328319
H	2.237061	-3.898102	-0.175252
C	-3.742685	-0.926698	0.005346
H	-4.607965	-0.777472	-0.646756
C	0.030624	-0.960793	-0.568160
H	-0.742436	-0.313148	-0.975532

O	0.539537	-0.352169	0.559135	O	0.549841	-0.423142	0.679587
C	2.800224	0.543254	0.829158	C	2.948916	0.132809	0.741043
C	4.004076	0.946185	0.227301	C	4.187604	0.084834	0.087447
C	2.832629	0.061290	2.146640	C	2.918069	0.133073	2.141371
C	5.205018	0.896909	0.937916	C	5.374681	0.048970	0.822991
H	4.009410	1.282554	-0.805329	H	4.232867	0.066370	-0.997627
C	4.032876	0.014501	2.855665	C	4.104368	0.091413	2.875770
H	1.911447	-0.275502	2.610908	H	1.961107	0.157702	2.653311
C	5.223391	0.435674	2.255587	C	5.336799	0.052054	2.218880
H	6.126871	1.211399	0.456328	H	6.327664	0.010550	0.302413
H	4.038847	-0.352294	3.878652	H	4.064773	0.089311	3.961762
H	6.157976	0.396859	2.808281	H	6.260281	0.019414	2.790420
C	-1.460885	-2.767898	-0.444352	C	-1.992391	-2.471835	-0.367640
H	-1.609152	-3.657381	-1.065334	H	-2.233416	-3.312488	-1.026030
C	2.457037	-1.489379	-1.458605	C	2.201682	-2.049785	-1.162969
O	3.509853	-1.495984	-2.252512	O	2.556154	-2.715765	-2.267836
C	1.476622	-0.429602	-1.445590	C	1.401479	-0.769494	-1.263115
C	1.366127	0.357523	-2.741604	C	1.387644	-0.233175	-2.691011
H	2.334231	0.783907	-3.024745	H	2.398702	0.002483	-3.039400
H	1.043273	-0.299805	-3.557617	H	0.970466	-0.986936	-3.365509
H	0.644041	1.170313	-2.647584	H	0.783032	0.672709	-2.763470
C	1.507973	0.597702	0.080607	C	1.650905	0.228623	-0.030858
C	0.874540	1.939882	-0.146871	C	1.248124	1.674607	-0.360132
C	-0.528530	2.010972	-0.106944	C	-0.068751	2.064191	-0.097477
C	1.576363	3.119400	-0.457893	C	2.096769	2.585240	-0.999617
C	-1.251129	3.164940	-0.406754	C	-0.599157	3.282029	-0.528791
H	-1.058792	1.118622	0.179212	H	-0.687517	1.364969	0.443618
C	0.871657	4.290324	-0.734359	C	1.597908	3.827225	-1.400622
H	2.660711	3.130900	-0.479474	H	3.133546	2.331976	-1.199509
C	-0.528723	4.324090	-0.725241	C	0.259199	4.170082	-1.191859
H	1.421738	5.198040	-0.967900	H	2.256541	4.530857	-1.902524
H	-1.037489	5.251833	-0.964890	H	-0.106036	5.125979	-1.555183
C	-3.268405	2.016976	0.529180	C	-2.742534	2.567822	0.583960
O	-3.517895	2.193762	1.703727	O	-2.917590	2.732471	1.774045
C	-2.791835	3.104035	-0.434365	C	-2.095919	3.591315	-0.348570
H	-3.089116	2.790745	-1.443518	H	-2.572347	3.473327	-1.330776
C	-3.482010	4.434511	-0.101673	C	-2.370344	5.010859	0.174029
H	-3.191983	4.787486	0.891934	H	-1.919514	5.153376	1.159855
H	-3.223931	5.201806	-0.836112	H	-1.963559	5.761510	-0.508188
H	-4.569580	4.312916	-0.118408	H	-3.447416	5.185425	0.260760

^{1}Oxe$_{2}^{*}$

O	-3.134875	1.301913	-0.035992
C	-3.489898	0.195678	0.823093
H	-2.685337	0.051348	1.550830
H	-4.403556	0.440060	1.372939
O	-2.616406	-1.370226	-0.883327
C	-3.876841	-2.290511	0.901934
C	-2.433102	-2.804555	0.979569

^{1}IM$_{2}^{*}$

O	3.123459	0.853545	0.055954
C	3.230889	-0.052936	-1.056738
H	2.271066	-0.027962	-1.584735
H	4.013957	0.280800	-1.741607
O	2.789802	-1.853759	0.598440
C	3.197118	-2.505123	-1.642794
C	1.746743	-2.835580	-1.279514

H	-4.283852	-2.028033	1.887228	H	3.287386	-2.099437	-2.658295
H	-2.366882	-3.859492	1.250767	H	1.443737	-3.809848	-1.658780
H	-1.849321	-2.225647	1.703213	H	1.055391	-2.071782	-1.646627
O	-4.735541	-3.203255	0.223238	O	3.944614	-3.704415	-1.494997
H	-4.776334	-4.016972	0.751672	H	4.871552	-3.514476	-1.714293
N	-0.474920	-2.291639	-0.587630	N	0.515046	-2.362170	0.900372
C	0.373448	-3.357485	-0.354668	C	-0.624079	-3.200954	0.669018
O	-0.005163	-4.469666	0.019607	O	-0.533884	-4.191826	-0.020593
N	1.707381	-3.072571	-0.585347	N	-1.768589	-2.800159	1.308042
H	2.329380	-3.866406	-0.482007	H	-2.588804	-3.374973	1.138063
C	-3.723612	-1.061679	-0.008870	C	3.560277	-1.459326	-0.569647
H	-4.605814	-0.933190	-0.642552	H	4.608687	-1.522021	-0.266938
C	0.037810	-0.969082	-0.658664	C	0.455598	-1.281283	1.660793
H	-0.748152	-0.327044	-1.052359	H	1.382893	-0.733903	1.769110
O	0.532202	-0.447620	0.608100	O	-0.890053	-0.366597	-0.714132
C	2.907995	0.173127	0.732928	C	-3.087768	0.501738	-0.979653
C	4.153431	0.329412	0.107444	C	-4.123888	1.340701	-0.499068
C	2.866387	-0.046084	2.115551	C	-3.485959	-0.643268	-1.715668
C	5.333589	0.271243	0.852949	C	-5.463537	1.070624	-0.772894
H	4.212725	0.480175	-0.966037	H	-3.880897	2.189765	0.130746
C	4.046402	-0.104229	2.859701	C	-4.823049	-0.905072	-1.993719
H	1.907206	-0.180663	2.604624	H	-2.708995	-1.315433	-2.065012
C	5.284105	0.057842	2.231422	C	-5.829716	-0.047470	-1.530654
H	6.290270	0.390189	0.351939	H	-6.230828	1.732782	-0.377414
H	3.997522	-0.279709	3.930998	H	-5.087192	-1.785842	-2.575591
H	6.201888	0.013192	2.811098	H	-6.874904	-0.252880	-1.745044
C	-1.927039	-2.535750	-0.444146	C	1.807474	-2.791276	0.254079
H	-2.169044	-3.375311	-1.104388	H	2.031092	-3.766516	0.695813
C	2.159686	-1.986750	-1.343368	C	-1.947164	-1.662608	2.088547
O	3.437155	-2.018927	-1.684977	O	-3.033681	-1.375179	2.563285
C	1.398278	-0.705068	-1.352028	C	-0.724768	-0.870714	2.303008
C	1.384541	-0.057761	-2.737681	C	-0.768228	0.344320	3.142199
H	2.389076	0.259658	-3.035055	H	0.106213	0.402880	3.798459
H	1.025378	-0.777968	-3.479624	H	-0.730236	1.229186	2.486821
H	0.730700	0.816800	-2.756191	H	-1.688724	0.380940	3.724290
C	1.613780	0.274889	-0.043163	C	-1.652296	0.681023	-0.691820
C	1.168646	1.716304	-0.312782	C	-1.047831	1.988162	-0.407791
C	-0.172910	2.045047	-0.078611	C	0.286048	1.997018	0.075689
C	2.000001	2.694533	-0.875676	C	-1.623569	3.264450	-0.659807
C	-0.734814	3.264591	-0.462466	C	1.014019	3.162554	0.319660
H	-0.783297	1.299323	0.405589	H	0.754915	1.034675	0.219554
C	1.465135	3.934204	-1.231321	C	-0.908445	4.429924	-0.413743
H	3.052471	2.497898	-1.051077	H	-2.615161	3.341816	-1.090997
C	0.108312	4.217758	-1.050838	C	0.407928	4.403278	0.077406
H	2.112706	4.686781	-1.673186	H	-1.373730	5.390166	-0.626164
H	-0.280127	5.178526	-1.374066	H	0.937608	5.333367	0.250449
C	-2.864001	2.461345	0.613380	C	3.169621	2.178907	-0.257875
O	-3.060099	2.610369	1.802156	O	3.640680	2.598919	-1.294296
C	-2.246307	3.513777	-0.305171	C	2.475753	3.027800	0.799777
H	-2.703131	3.381061	-1.294857	H	2.479341	2.457164	1.735174

C	-2.587343	4.918133	0.218712	C	3.218114	4.349970	1.012100
H	-2.144167	5.081620	1.204775	H	3.291787	4.915662	0.079079
H	-2.218255	5.688525	-0.462788	H	2.702078	4.965966	1.754409
H	-3.671529	5.040486	0.305543	H	4.233368	4.161541	1.375983

ISC $^{S_1/T_1}_{2}(a)$

O	3.161280	0.780018	0.155652	O	-3.096444	1.300522	-0.086878
C	3.246370	-0.165939	-0.926652	C	-3.501506	0.200495	0.756580
H	2.294169	-0.124458	-1.468464	H	-2.743866	0.061669	1.532777
H	4.052022	0.116603	-1.608273	H	-4.443007	0.449831	1.255541
O	2.646305	-1.926279	0.717729	O	-2.589721	-1.415461	-0.909833
C	3.249397	-2.624710	-1.477001	C	-3.856015	-2.287622	0.876597
C	1.778770	-2.995754	-1.203839	C	-2.395039	-2.724795	1.072778
H	3.372859	-2.211536	-2.480999	H	-4.318703	-2.027676	1.837744
H	1.534688	-3.994360	-1.562559	H	-2.274354	-3.766432	1.362501
H	1.100591	-2.274549	-1.670002	H	-1.864753	-2.088423	1.785003
O	4.137880	-3.728998	-1.419165	O	-4.604932	-3.266752	0.180945
H	4.126537	-4.105941	-0.524046	H	-4.689140	-4.047686	0.752891
N	0.344097	-2.426949	0.827178	N	-0.449443	-2.225752	-0.461972
C	-0.748203	-3.300462	0.558836	C	0.500209	-3.330354	-0.107059
O	-0.591299	-4.331352	-0.062765	O	0.008174	-4.358138	0.330241
N	-1.951025	-2.882300	1.070853	N	1.746656	-2.923890	-0.272642
H	-2.744957	-3.483278	0.870501	H	2.441422	-3.607579	0.009089
C	3.518355	-1.563595	-0.390328	C	-3.715056	-1.076335	-0.056687
H	4.538813	-1.630756	-0.005493	H	-4.578176	-0.974894	-0.717147
C	0.204133	-1.310412	1.542457	C	0.025072	-0.857103	-0.620777
H	1.111668	-0.743826	1.702049	H	-0.807812	-0.263419	-0.986247
O	-0.813677	-0.219704	-0.874908	O	0.523041	-0.386516	0.639555
C	-3.006799	0.677610	-0.989640	C	2.936197	0.146036	0.715800
C	-4.006821	1.520471	-0.441260	C	4.168970	0.101255	0.051334
C	-3.451495	-0.449717	-1.728505	C	2.911439	0.106338	2.116146
C	-5.360247	1.266677	-0.651553	C	5.359240	0.032278	0.779861
H	-3.725164	2.356702	0.188847	H	4.200262	0.108418	-1.033367
C	-4.804255	-0.696925	-1.934497	C	4.100680	0.029477	2.842040
H	-2.703158	-1.120360	-2.137501	H	1.958416	0.132446	2.636233
C	-5.775694	0.161534	-1.403313	C	5.328492	-0.005947	2.175381
H	-6.099403	1.931568	-0.210019	H	6.309406	-0.000534	0.253345
H	-5.106954	-1.567361	-2.512530	H	4.068062	0.000973	3.928029
H	-6.832441	-0.032707	-1.563150	H	6.254764	-0.065332	2.740006
C	1.689862	-2.875450	0.324197	C	-1.855984	-2.485026	-0.383081
H	1.865279	-3.828763	0.833716	H	-2.038077	-3.411672	-0.953223
C	-2.204333	-1.733714	1.818477	C	2.208827	-1.932517	-1.424100
O	-3.329168	-1.471143	2.217115	O	2.470142	-2.493764	-2.519292
C	-1.018830	-0.908567	2.084897	C	1.363863	-0.652260	-1.330791
C	-1.149247	0.300153	2.933564	C	1.277274	-0.001473	-2.707309
H	-0.874266	0.058285	3.971093	H	2.269714	0.313913	-3.044858
H	-0.482841	1.096340	2.591623	H	0.912296	-0.735893	-3.429840
H	-2.183538	0.647110	2.938863	H	0.617973	0.868856	-2.713020
C	-1.564396	0.837790	-0.756807	C	1.646000	0.286339	-0.052170

C	-0.921212	2.108488	-0.405690	C	1.216474	1.742768	-0.292720
C	0.409151	2.056945	0.079246	C	-0.112674	2.089053	-0.025687
C	-1.467795	3.404054	-0.606393	C	2.042766	2.699197	-0.891773
C	1.172520	3.192584	0.357312	C	-0.681050	3.295555	-0.434465
H	0.846284	1.077103	0.202478	H	-0.719060	1.363249	0.492724
C	-0.718707	4.539874	-0.321769	C	1.507009	3.936920	-1.260540
H	-2.459098	3.521986	-1.028165	H	3.087755	2.482310	-1.092889
C	0.599082	4.455962	0.155749	C	0.154382	4.229615	-1.063379
H	-1.158189	5.519837	-0.493752	H	2.147650	4.675687	-1.734870
H	1.157574	5.364465	0.352044	H	-0.239110	5.180365	-1.410110
C	3.283421	2.090746	-0.195284	C	-2.824554	2.447614	0.596031
O	3.785226	2.455191	-1.238252	O	-3.037628	2.558861	1.785040
C	2.631090	3.006934	0.832705	C	-2.193297	3.535470	-0.274516
H	2.618143	2.472443	1.789497	H	-2.643427	3.449198	-1.272141
C	3.433621	4.302086	0.990411	C	-2.530927	4.916967	0.311573
H	3.508109	4.838181	0.040206	H	-2.111160	5.022021	1.315623
H	2.964357	4.960310	1.727250	H	-2.128408	5.712572	-0.320479
H	4.448594	4.079872	1.335402	H	-3.614947	5.053854	0.376355