Supplementary information for

Nonadiabatic molecular dynamic simulations for ultrafast photo-induced ring-opening and isomerization reactions of 2,2-diphenyl-2H-chromene

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Fig. S3--HOOP motions with respect to time evolution of rC5O6, φH24C4C5C12 and φH23C4C5C12 for two trajectories starting from FC-T.

Fig. S4--HOOP motions with respect to time evolution of rC5O6, φH24C4C5C12 and φH23C4C5C12 for two trajectories starting from FC-C.

Fig. S5--A typical ring-opening reactive trajectory starting from FC-T goes via FC-T→CI-S_1/S_0-T→S_0-CC-C→S_0-TC pathway as function of time.
Fig. S6--A typical ring-opening reactive trajectory starting from FC-C goes via FC-C→CI-S_1/S_0-C→S_0-CC-T→S_0-TC pathway as function of time.

Table S5--Cartesian coordinates (in Å) for geometries optimized in Table S1 at CAM-B3LYP-D3/def2-SVP level of theory.

Table S6--Cartesian coordinates (in Å) for geometries optimized in Table S1 at CAM-B3LYP-D3/def2-SV(P) level of theory.

Table S1. S_1 state configurations and S_0 and S_1 state relative energies calculated by (TD)-CAM-B3LYP-D3/def2-SVP and SDSPT2/def2-SVP on the basis of (TD)-CAM-B3LYP-D3 optimized geometries.

State	S_1 configuration weight (%)		E_{TDDFT} (eV)		E_{SDSPT2} (eV)	
	DFT	SDSPT2	S_0	S_1	S_0	S_1
S_0-C	HOMO→LUMO (83.2)	HOMO-1→LUMO (36.8) HOMO→LUMO+1 (22.7)	0.07	4.68	0.08	4.80
CI-S_1/S_0-C	HOMO→LUMO (94.2)	HOMO→LUMO (73.0)	3.04	3.06	2.84	3.33
S_0-CC-C	HOMO-2→LUMO (48.0) HOMO→LUMO (34.6)	HOMO-1→LUMO (61.1)	1.25	4.03	1.10	3.82
S_1-C	HOMO→LUMO (92.8)	HOMO-1→LUMO (34.1) HOMO→LUMO+1 (16.7)	0.50	4.27	0.44	4.64
S_0-TC	HOMO-2→LUMO (56.1) HOMO-1→LUMO (33.9)	HOMO→LUMO (42.9) HOMO-1→LUMO (10.1)	0.93	3.83	0.72	4.01
S_0-T	HOMO→LUMO (80.2)	HOMO-1→LUMO (38.3) HOMO→LUMO+1 (24.4)	0.00	4.67	0.00	4.77
CI-S_1/S_0-T	HOMO→LUMO (96.7)	HOMO→LUMO (73.4)	2.56	2.59	2.25	2.69
S_0-CC-T	HOMO-2→LUMO (47.2) HOMO→LUMO (35.3)	HOMO-1→LUMO (61.8)	1.24	4.02	1.10	3.82
S_1-T	HOMO→LUMO (90.9)	HOMO-1→LUMO (34.8) HOMO→LUMO+1 (16.8)	0.35	4.34	0.32	4.57
S_0-TT	HOMO-2→LUMO (75.9)	HOMO→LUMO (38.1) HOMO-1→LUMO (11.3)	0.95	3.96	0.72	4.22

Table S2a. Optimized geometry structures of ten critical points for DPC (bond length in angstrom and dihedral angles in degree) [a] by CAM-B3LYP-D3/def2-SVP in terms of internal coordinates.

	S_0-C	S_1-C	CI-S_1/S_0-C	S_0-CC-C	S_0-T	S_1-T	CI-S_1/S_0-T	S_0-CC-T	S_0-TC	S_0-TT
r_{O6C5}	1.435	1.459	2.753	3.161	1.434	1.444	2.564	2.935	4.147	5.032
r_{O6C1}	1.354	1.319	1.232	1.218	1.357	1.323	1.247	1.222	1.225	1.221
r_{C4C5}	1.516	1.475	1.465	1.343	1.516	1.478	1.468	1.356	1.361	1.360
r_{C3C4}	1.334	1.389	1.360	1.466	1.335	1.388	1.348	1.446	1.434	1.436
r_{C2C3}	1.457	1.409	1.432	1.355	1.459	1.408	1.474	1.368	1.370	1.364
r_{C1C2}	1.402	1.459	1.473	1.502	1.403	1.457	1.454	1.495	1.495	1.499
r_{H29O6}	3.349	2.636	3.792	4.505	2.660	2.903	3.214	2.960	6.564	6.418
r_{H29C11}	2.533	2.900	2.557	2.619	2.898	2.678	2.729	2.829	2.900	2.825
r_{H33C4}	2.554	2.547	2.575	2.699	2.497	2.543	2.642	2.876	2.966	2.919
r_{H38O6}	2.336	2.607	2.408	2.398	2.312	2.369	2.763	4.108	3.776	6.567
r_{H34C12}	3.025	2.540	3.026	3.517	2.666	2.740	2.758	2.679	2.613	2.671
θ_{C5C4C3}	121.7	120.7	134.1	126.3	120.4	122.1	127.4	129.7	124.3	125.2
θ_{C4C3C2}	120.5	120.0	134.6	130.5	120.0	120.8	125.2	132.8	127.6	126.9
θ_{C3C2C1}	117.2	118.1	124.2	122.6	117.0	117.7	117.1	124.1	123.2	116.5
θ_{C5O6C1}	121.6	121.9	113.0	102.0	118.5	124.5	97.9	106.2	94.9	77.2
$\varphi_{C13C12C5C4}$	-148.3	178.9	177.1	156.2	174.5	-166.3	154.6	142.0	126.7	131.8
$\varphi_{C18C11C5C4}$	57.6	98.5	99.6	81.8	80.1	78.6	143.0	133.9	151.0	144.2
$\varphi_{O6C5C4C3}$	-20.9	-24.9	-14.6	-69.8	28.4	3.7	41.9	49.4	-166.0	2.0
$\varphi_{C5C4C3C2}$	3.3	12.1	5.4	70.8	-1.5	0.4	-3.8	-43.8	176.0	173.0
$\varphi_{C4C3C2C1}$	8.3	0.7	9.9	5.2	-13.5	-1.9	-36.8	-7.0	-1.7	177.7
$\varphi_{C2C1O6C5}$	-19.9	-16.3	-13.1	-25.6	31.1	5.9	52.1	21.0	-0.4	0.9
$\varphi_{C4C12C11C5}$	-34.1	-32.6	-9.2	-1.0	-32.8	-31.9	-3.2	-1.6	-0.3	-0.4

[a]The CIs are optimized by BDF program with inclusion of RI.

Table S2b. Optimized geometry structures of ten critical points for DPC (bond length in angstrom and dihedral angles in degree)[a] by CAM-B3LYP-D3/def2-SV(P) in terms of internal coordinates.

	S_0-C	S_1-C	CI-S_1/S_0-C	S_0-CC-C	S_0-T	S_1-T	CI-S_1/S_0-T	S_0-CC-T	S_0-TC	S_0-TT
r_{O6C5}	1.435	1.459	2.870	3.073	1.434	1.444	2.567	2.935	4.150	5.032
r_{O6C1}	1.354	1.319	1.221	1.219	1.356	1.323	1.246	1.222	1.224	1.221
r_{C4C5}	1.516	1.476	1.485	1.348	1.516	1.478	1.471	1.357	1.362	1.361
r_{C3C4}	1.334	1.390	1.351	1.458	1.336	1.388	1.345	1.447	1.435	1.437
r_{C2C3}	1.458	1.409	1.465	1.360	1.459	1.409	1.477	1.368	1.370	1.365
r_{C1C2}	1.402	1.459	1.467	1.499	1.403	1.457	1.454	1.495	1.495	1.499
r_{H29O6}	3.319	2.643	3.839	4.900	2.664	2.903	3.215	2.951	6.578	6.420
r_{H29C11}	2.544	2.893	2.564	2.496	2.897	2.679	2.729	2.830	2.893	2.823
r_{H33C4}	2.544	2.552	2.570	2.663	2.497	2.543	2.642	2.877	2.961	2.917
r_{H38O6}	2.345	2.606	2.345	2.580	2.312	2.369	2.764	4.097	2.804	6.568
r_{H34C12}	2.988	2.542	3.060	3.717	2.669	2.741	2.758	2.682	2.617	2.673
θ_{C5C4C3}	121.8	120.7	127.7	127.3	120.4	122.1	127.5	129.6	124.3	125.2
θ_{C4C3C2}	120.5	120.2	138.5	131.8	120.0	120.8	125.2	132.7	127.6	127.0
θ_{C3C2C1}	117.2	118.1	123.9	123.3	117.0	117.7	117.0	124.0	123.2	116.5
θ_{C5C6O1}	121.7	122.0	108.1	103.3	118.5	124.5	97.8	106.3	94.9	77.3
$\varphi_{C13C12C5C4}$	-149.9	179.3	179.9	152.1	174.7	-166.2	154.5	133.9	127.3	132.1
$\varphi_{C18C11C5C4}$	59.6	98.4	97.0	66.2	79.9	78.6	143.1	141.9	150.5	144.1
$\varphi_{O6C5C4C3}$	-20.5	-24.8	-13.9	-62.0	28.4	3.8	41.9	49.5	-165.2	2.1
$\varphi_{C5C4C3C2}$	3.2	12.2	5.5	59.7	-1.6	0.4	-3.8	-44.0	175.8	172.9
$\varphi_{C4C3C2C1}$	8.0	0.6	20.7	6.2	-13.4	-1.9	-36.9	-6.9	-1.8	177.7
$\varphi_{C2C1O6C5}$	-19.7	-16.1	-12.8	-24.6	31.1	6.0	52.1	20.8	-0.4	0.9
$\varphi_{C4C12C11C5}$	-34.2	-32.6	-11.4	-1.3	-32.8	-31.9	-3.1	-1.6	-0.3	-0.4

[a]The CIs are optimized by BDF program without inclusion of RI.

Table S3. Potential energies in eV for optimized geometries in Table S1.

Basis set	Geometries	S_0	S_1	S_2	S_3
def2-SVP	S_0-C	0.07	4.68	5.28	5.57
	S_1-C	0.50	4.27	5.25	5.76
	CI-S_1/S_0-C	3.04	3.06	5.00	5.22
	S_0-CC	1.24	4.03	4.56	5.07
	S_0-TC	0.93	3.83	4.15	4.97
	S_0-T	0.00	4.67	5.28	5.51
	S_1-T	0.35	4.34	5.23	5.75
	CI-S_1/S_0-T	2.56	2.59	4.17	5.11
	S_0-CC-T	1.24	4.02	4.55	5.06
	S_0-TT	0.95	3.96	4.22	5.10
def2-SV(P)	S_0-C	0.07	4.68	5.28	5.58
	S_1-C	0.50	4.27	5.26	5.76
	CI-S_1/S_0-C	3.05	3.06	5.00	5.23
	S_0-CC	1.24	4.02	4.55	5.07
	S_0-TC	0.93	3.83	4.15	4.98
	S_0-T	0.00	4.67	5.28	5.52
	S_1-T	0.35	4.35	5.23	5.75
	CI-S_1/S_0-T	2.56	2.59	4.17	5.11
	S_0-CC-T	1.24	4.02	4.55	5.06
	S_0-TT	0.95	3.96	4.22	5.09

Table S4. Average lifetimes and standard deviations (in fs) of each dynamics steps for observed DPC reaction mechanisms.

Mechanism	No.	S_1/S_0 hop	S_0-CC-T/C	S_0 product
FC-T→CI-S_1/S_0-T→S_0-CC-T→S_0-TC	162	124.3 (100.2)	161.8 (107.3)	1305.7(623.3)
FC-T→CI-S_1/S_0-T→S_0-CC-C→S_0-TC	13	118.7 (24.3)	195.2 (41.6)	867.5 (292.5)
FC-T→CI-S_1/S_0-C→S_0-CC-C→S_0-TC	6	615.5 (136.0)	636.5 (134.3)	979.8 (112.4)
FC-T→CI-S_1/S_0-T→S_0-T	19	150.5 (45.3)		209.5 (51.0)
FC-C→CI-S_1/S_0-C→S_0-CC-C→S_0-TC	69	439.8 (214.0)	517.3 (221.9)	1125.7 (370.3)
FC-C→CI-S_1/S_0-C→S_0-CC-T→S_0-TC	18	380.2 (195.0)	580.8 (198.8)	1248.7 (554.0)
FC-C→CI-S_1/S_0-T→S_0-CC-T→S_0-TC	27	457.9 (225.3)	572.6 (250.5)	1380.4 (338.9)
FC-C→CI-S_1/S_0-C→ S_0-C	35	566.9 (259.8)		673.3 (277.1)
FC-C→CI-S_1/S_0-T→S_0-T	1	317.0		397.5

Fig. S1 DPC-C↔DPC-T isomerization potential energy curves calculated by CAM-B3LYP-D3/def2-SVP on (a) S_0 state (MEP) and (b) S_1 state (LIIC).

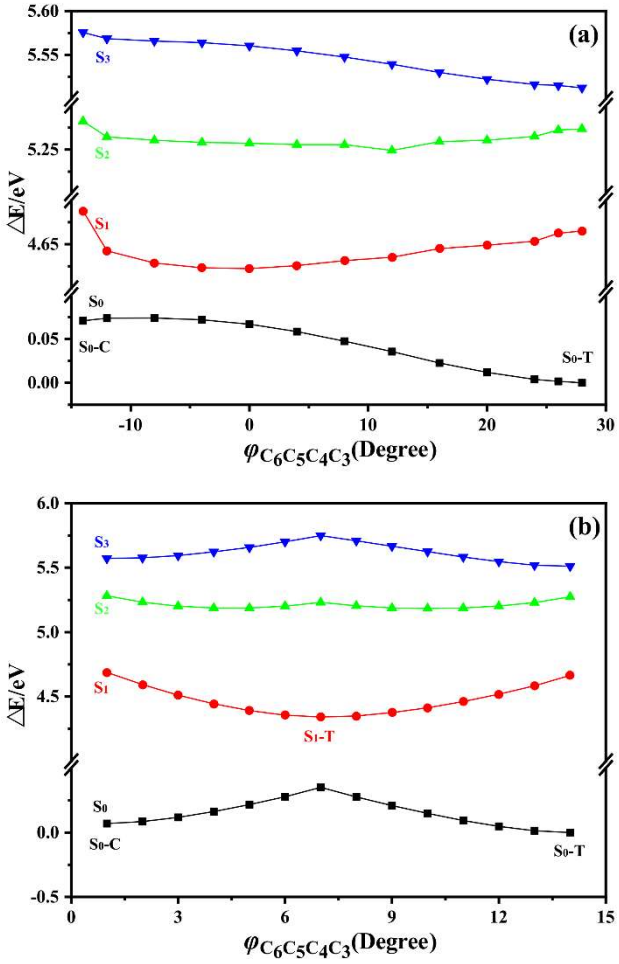

Fig. S2 Hopping-spot distributions at CI-S_1/S_0-C and CI-S_1/S_0-T with respect to $\varphi_{H24C4C5C3}$ and $\varphi_{H23C3C4C2}$ dihedral angles for trajectories starting from (a) FC-T and (b) FC-C.

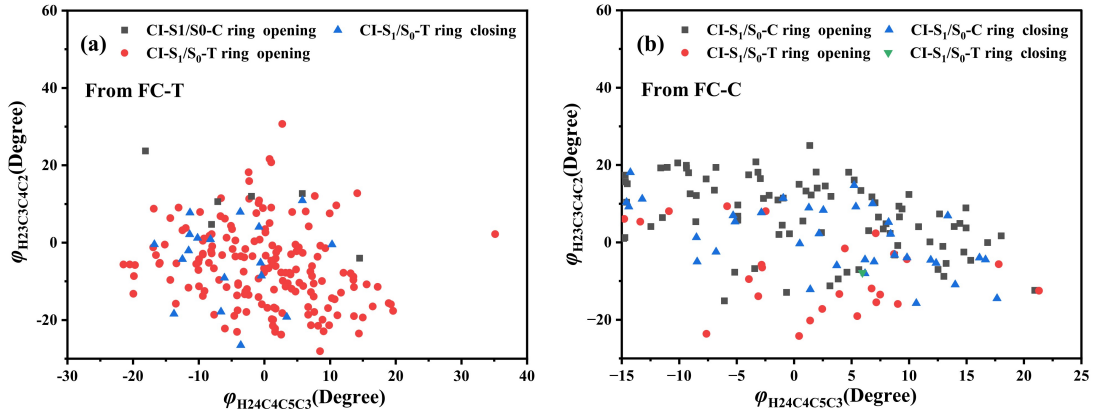

Fig. S3 HOOP motions with respect to time evolution of r_{C5O6}, $\varphi_{H24C4C5C12}$ and $\varphi_{H23C4C5C12}$ for two trajectories starting from FC-T. (a) one trajectory and (b) another.

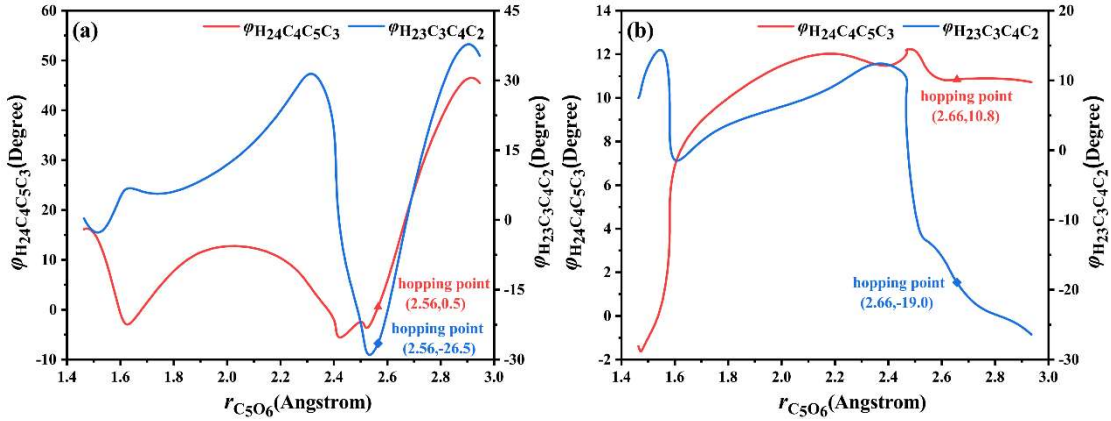

Fig. S4 The same as in Fig. S3 except for trajectories starting from FC-C.

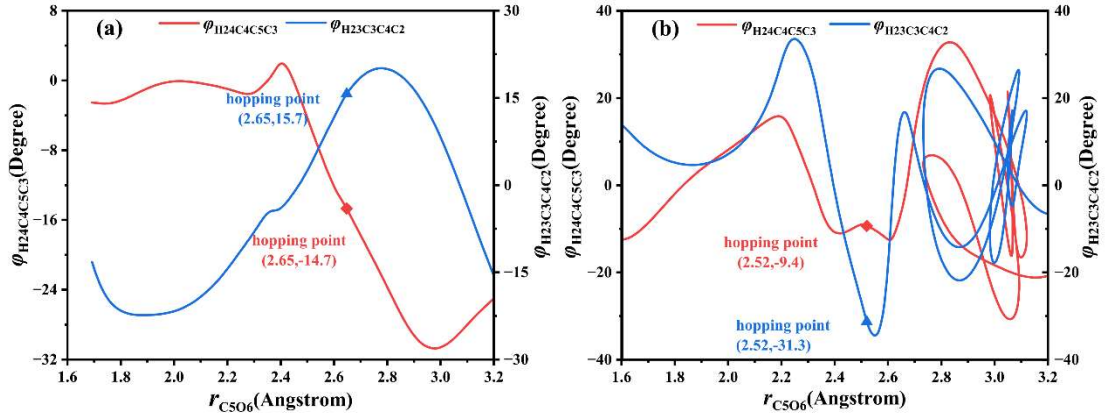

Fig. S5 A typical ring-opening reactive trajectory starting from FC-T goes via FC-T→CI-S_1/S_0-T→S_0-CC-C→S_0-TC pathway as function of time. (a) Potential energy profiles of the S_0 and S_1 states, (b) evolution of r_{C5O6}, r_{H38O6} and r_{H29O6}, (c) $\varphi_{O6C5C4C3}$, $\varphi_{C5C4C3C2}$ and $\varphi_{C4C3C2C1}$, and (d) $\varphi_{C18C11C5C4}$, $\varphi_{C17C12C5C4}$ and $\varphi_{H24C4C5C12}$.

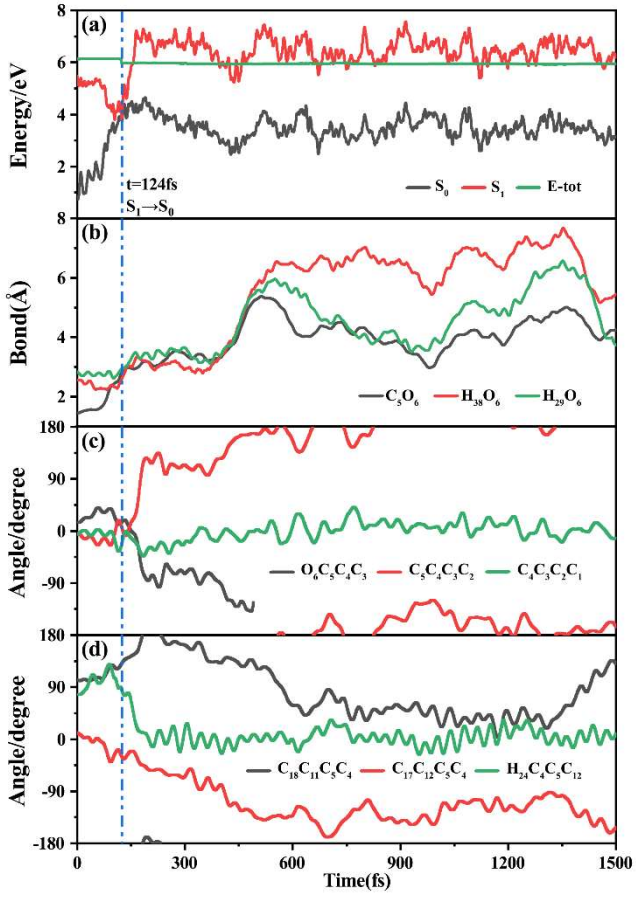

Fig. S6 A typical ring-opening reactive trajectory starting from FC-C goes via FC-C→CI-S_1/S_0-C→S_0-CC-T→S_0-TC pathway as function of time. (a) Potential energy profiles of the S_0 and S_1 states, (b) evolution of r_{C5O6}, r_{H38O6} and r_{H29O6}, (c) $\varphi_{O6C5C4C3}$, $\varphi_{C5C4C3C2}$ and $\varphi_{C4C3C2C1}$, and (d) $\varphi_{C18C11C5C4}$, $\varphi_{C17C12C5C4}$ and $\varphi_{H24C4C5C12}$.

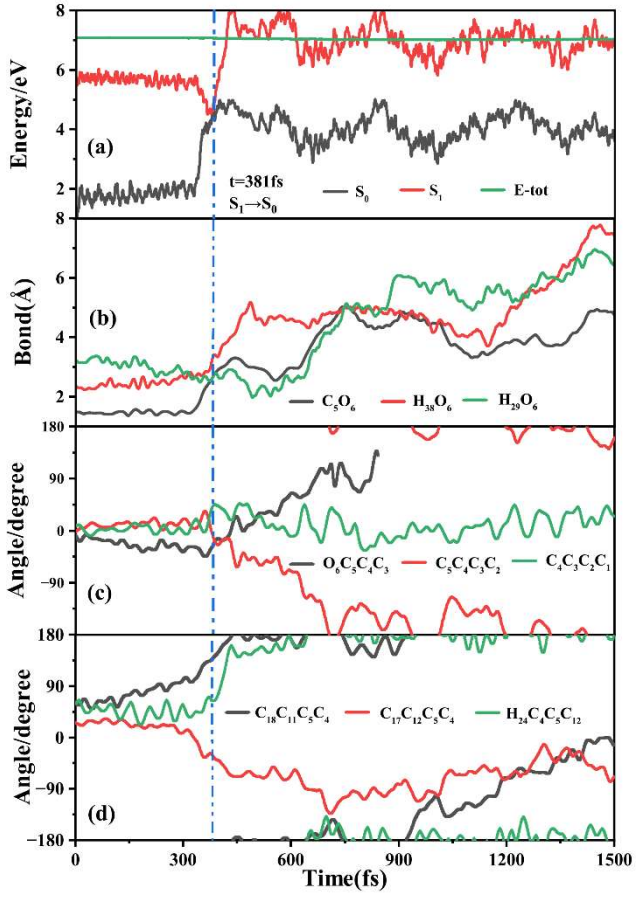

Table S5. Cartesian coordinates (in Å) for geometries optimized in Table S1 at CAM-B3LYP-D3/def2-SVP level of theory.

S_0-C				S_0-T			
C	1.505715	1.994850	0.978185	C	0.006144	2.180664	1.112111
C	1.750575	3.354294	0.829815	C	0.048473	3.551322	0.853578
C	1.113063	4.074865	-0.179909	C	-0.233596	4.031014	-0.419469
C	0.235890	3.420930	-1.037427	C	-0.561332	3.134925	-1.437762
C	-0.007297	2.055283	-0.890098	C	-0.610385	1.772693	-1.176557
C	0.622672	1.331354	0.119969	C	-0.328475	1.282876	0.102805
C	0.359917	-0.165536	0.305587	C	-0.390017	-0.232913	0.320174
C	-0.157341	-0.386767	1.713292	C	0.063027	-0.646676	1.706006
C	-1.458307	-0.533690	1.967217	C	1.339472	-0.964040	1.933286
C	-2.426721	-0.556693	0.878332	C	2.301301	-0.946030	0.836317
C	-1.920758	-0.598300	-0.428905	C	1.782375	-0.876171	-0.465672
O	-0.588926	-0.609741	-0.674564	O	0.442724	-0.848108	-0.672280
C	1.609227	-1.004247	0.031552	C	-1.802409	-0.760307	0.078333
C	2.609562	-0.556239	-0.832099	C	-2.900873	-0.078435	0.606481
C	3.704200	-1.365055	-1.125984	C	-4.187750	-0.581286	0.445806
C	3.811083	-2.632626	-0.560326	C	-4.392298	-1.769987	-0.250977
C	2.812317	-3.090300	0.295728	C	-3.300790	-2.451010	-0.780802
C	1.718008	-2.281008	0.585317	C	-2.010939	-1.951995	-0.613932
C	-2.782042	-0.679528	-1.520092	C	2.625133	-0.906263	-1.571705
C	-4.157218	-0.699929	-1.310486	C	4.000684	-0.992995	-1.381952
C	-4.678224	-0.645701	-0.017739	C	4.535768	-1.054629	-0.095383
C	-3.810333	-0.580936	1.066637	C	3.684845	-1.036748	1.003816
H	2.022649	1.440529	1.764124	H	0.245715	1.810720	2.109504
H	2.446134	3.856511	1.505369	H	0.311470	4.244590	1.655356
H	1.305630	5.143144	-0.297706	H	-0.196191	5.103267	-0.623551
H	-0.265689	3.973962	-1.834215	H	-0.782055	3.504459	-2.441376
H	-0.685999	1.545074	-1.571459	H	-0.867456	1.067673	-1.969082
H	0.579176	-0.368343	2.516992	H	-0.686853	-0.659556	2.498449
H	-1.821210	-0.644046	2.991634	H	1.682742	-1.251245	2.930040
H	2.534577	0.435101	-1.279623	H	-2.749387	0.862922	1.138466
H	4.479980	-1.000699	-1.802608	H	-5.037634	-0.036039	0.861417
H	4.671598	-3.265106	-0.788079	H	-5.402621	-2.162814	-0.382545
H	2.883461	-4.085268	0.739523	H	-3.451475	-3.383592	-1.328736
H	0.930418	-2.649538	1.245231	H	-1.153313	-2.482265	-1.025754
H	-2.351759	-0.728622	-2.521361	H	2.183712	-0.857969	-2.567913
H	-4.829699	-0.757857	-2.168731	H	4.662745	-1.009237	-2.250186
H	-5.757462	-0.660273	0.142724	H	5.615580	-1.121848	0.048703
H	-4.202688	-0.551226	2.085989	H	4.091352	-1.097901	2.016353

S_0-CC-C				S_0-CC-T			
C	0.351150	1.742348	-0.988102	C	-0.005272	0.013049	0.008079
C	0.969523	2.929762	-0.612520	C	-0.014522	0.014066	1.398242
C	0.840107	3.400937	0.691576	C	1.184417	0.013425	2.107094
C	0.077338	2.686093	1.612574	C	2.393367	0.009815	1.415543
C	-0.544265	1.503130	1.235384	C	2.402963	0.014500	0.025348
C	-0.402046	1.007354	-0.067118	C	1.204162	0.024800	-0.700509
C	-1.034029	-0.273322	-0.450069	C	1.215193	0.049353	-2.182548
C	-0.380205	-1.238662	-1.143206	C	2.149070	0.785465	-2.835324
C	1.012344	-1.321708	-1.524278	C	2.407004	0.904023	-4.253282
C	2.176307	-1.067283	-0.852940	C	2.475576	-0.013420	-5.265182
C	2.248251	-0.744725	0.605210	C	2.423464	-1.493131	-5.058609
O	1.264241	-0.692592	1.327145	O	2.321287	-2.010575	-3.956722
C	-2.463614	-0.458040	-0.104408	C	0.146335	-0.693887	-2.883694
C	-3.357248	0.621060	-0.147379	C	-0.141838	-2.018544	-2.530146
C	-4.702204	0.442575	0.155580	C	-1.118010	-2.734779	-3.210297
C	-5.177319	-0.814787	0.521216	C	-1.831480	-2.135924	-4.246431
C	-4.297273	-1.892632	0.582078	C	-1.569975	-0.812202	-4.590974
C	-2.953379	-1.715774	0.272715	C	-0.589424	-0.096979	-3.912253
C	3.592741	-0.519018	1.150654	C	2.534500	-2.317877	-6.268349
C	4.702643	-0.626164	0.391124	C	2.702627	-1.777082	-7.492976
C	4.626206	-0.986718	-1.007370	C	2.798611	-0.345910	-7.677071
C	3.425212	-1.204688	-1.583672	C	2.701200	0.479514	-6.613577
H	0.445165	1.379403	-2.012557	H	-0.947518	0.014343	-0.542221
H	1.550102	3.494592	-1.344823	H	-0.966555	0.015345	1.933114
H	1.326167	4.332606	0.988473	H	1.176562	0.007134	3.199246
H	-0.028748	3.050892	2.636175	H	3.337684	-0.009053	1.963597
H	-1.122545	0.931965	1.962184	H	3.351560	-0.020862	-0.513133
H	-0.996702	-2.040504	-1.562687	H	2.749303	1.466411	-2.223181
H	1.154923	-1.721322	-2.536944	H	2.649972	1.930293	-4.559495
H	-2.990033	1.607910	-0.432881	H	0.432277	-2.494157	-1.734543
H	-5.385206	1.293233	0.106515	H	-1.319689	-3.771721	-2.934583
H	-6.231989	-0.952951	0.768337	H	-2.599553	-2.699533	-4.780361
H	-4.658076	-2.877398	0.886087	H	-2.137786	-0.330855	-5.389851
H	-2.260872	-2.555378	0.352929	H	-0.392253	0.942933	-4.176050
H	3.630977	-0.256158	2.208988	H	2.468881	-3.395477	-6.108267
H	5.685921	-0.445605	0.833137	H	2.776760	-2.424812	-8.370390
H	5.546536	-1.082699	-1.585776	H	2.953531	0.055148	-8.680006
H	3.362651	-1.479528	-2.639722	H	2.774392	1.561943	-6.748182

S_1-C				S_1-T			
C	1.586063	2.068759	0.305516	C	0.006787	-0.187910	-0.053684
C	1.587233	3.447093	0.149092	C	0.028541	-0.217318	1.334738
C	0.413646	4.127161	-0.184129	C	1.220529	-0.005103	2.026144
C	-0.762070	3.401593	-0.356840	C	2.391608	0.234722	1.311375
C	-0.777621	2.020808	-0.194711	C	2.376124	0.272480	-0.079194
C	0.402762	1.331085	0.129520	C	1.180376	0.069346	-0.773246
C	0.405596	-0.189362	0.373751	C	1.114764	0.147512	-2.300641
C	-0.136578	-0.345343	1.737086	C	0.570895	1.484303	-2.618728
C	-1.501344	-0.499405	1.943114	C	1.277210	2.404844	-3.380570
C	-2.356876	-0.763805	0.855551	C	2.551129	2.092182	-3.892937
C	-1.763952	-0.884848	-0.472174	C	3.115855	0.790903	-3.559504
O	-0.461267	-0.772890	-0.644887	O	2.460755	-0.057009	-2.783117
C	1.759989	-0.828815	0.108579	C	0.368255	-1.050763	-2.905397
C	2.303077	-0.727619	-1.175065	C	0.635608	-2.336629	-2.426443
C	3.528333	-1.310698	-1.470056	C	-0.001268	-3.438420	-2.983419
C	4.228873	-2.002557	-0.482235	C	-0.910530	-3.268694	-4.026832
C	3.689364	-2.113263	0.793962	C	-1.176511	-1.989775	-4.506831
C	2.454576	-1.534936	1.086447	C	-0.541588	-0.883404	-3.947040
C	-2.543585	-1.146864	-1.609945	C	4.373148	0.378083	-4.019659
C	-3.910091	-1.324689	-1.483429	C	5.137316	1.235045	-4.802841
C	-4.508560	-1.211415	-0.203637	C	4.616202	2.509302	-5.130195
C	-3.759023	-0.935699	0.926150	C	3.365292	2.926338	-4.693593
H	2.512870	1.554828	0.561198	H	-0.927290	-0.375009	-0.587194
H	2.520310	3.998469	0.285631	H	-0.893829	-0.418441	1.883810
H	0.417507	5.211947	-0.305743	H	1.237442	-0.035807	3.117088
H	-1.688670	3.916041	-0.621474	H	3.334174	0.387839	1.841461
H	-1.719539	1.489719	-0.336245	H	3.302144	0.449680	-0.626783
H	0.543499	-0.145120	2.563152	H	-0.384384	1.735521	-2.160392
H	-1.922623	-0.437423	2.947571	H	0.858065	3.393873	-3.571401
H	1.754552	-0.180567	-1.943591	H	1.348642	-2.469147	-1.611107
H	3.942680	-1.224097	-2.476676	H	0.212090	-4.438471	-2.600328
H	5.195050	-2.456699	-0.711426	H	-1.414452	-4.134588	-4.461380
H	4.227929	-2.658065	1.572104	H	-1.889879	-1.848480	-5.321409
H	2.026103	-1.645310	2.082545	H	-0.752874	0.123643	-4.310627
H	-2.031922	-1.211935	-2.571090	H	4.717608	-0.617030	-3.734406
H	-4.522151	-1.542950	-2.359122	H	6.122876	0.932114	-5.157184
H	-5.588078	-1.346594	-0.108268	H	5.215827	3.184257	-5.744991
H	-4.244336	-0.852878	1.900379	H	2.992090	3.915467	-4.965036

CI-S_1/S_0-C				CI-S_1/S_0-T			
C	-1.936154	-0.687134	-0.802375	C	1.410845	-1.235039	-0.857083
C	-2.349720	-0.631696	0.610768	C	1.869632	-1.525554	0.491929
C	-1.440626	-0.510581	1.710700	C	0.837142	-1.796481	1.508946
C	-0.110208	-0.252274	1.825795	C	-0.360207	-1.182727	1.584255
C	0.944574	0.110339	0.876068	C	-0.853656	-0.085992	0.741802
O	-0.755073	-0.650897	-1.151887	O	0.217158	-1.417191	-1.169877
C	-3.014260	-0.777961	-1.787518	C	2.385251	-0.738489	-1.797277
C	-4.322105	-0.814060	-1.427981	C	3.729440	-0.760986	-1.492938
C	-4.695645	-0.782953	-0.048669	C	4.152775	-1.175694	-0.219977
C	-3.729593	-0.703279	0.923123	C	3.222846	-1.529297	0.768424
C	1.113188	1.559219	0.612917	C	-2.222255	-0.192396	0.263459
C	1.955399	-0.807058	0.495914	C	-0.044028	1.082966	0.511446
C	2.927001	-0.445573	-0.473558	C	0.997231	1.447305	1.392671
C	3.943581	-1.316501	-0.816439	C	1.785408	2.566031	1.151497
C	4.037743	-2.568014	-0.199123	C	1.581193	3.340073	0.012138
C	3.078894	-2.953902	0.740298	C	0.580177	2.979267	-0.893661
C	2.041215	-2.100083	1.072238	C	-0.217267	1.874369	-0.652255
C	2.138662	2.252412	1.273591	C	-2.764982	-1.457636	-0.038234
C	2.304895	3.620181	1.086949	C	-4.088242	-1.584666	-0.439474
C	1.460912	4.308007	0.219210	C	-4.905059	-0.458814	-0.539065
C	0.447305	3.625544	-0.448537	C	-4.385419	0.800526	-0.242880
C	0.262038	2.262273	-0.245211	C	-3.060227	0.933959	0.149963
H	-1.944052	-0.615704	2.677396	H	1.071563	-2.544078	2.274590
H	0.243314	-0.219302	2.867972	H	-1.056213	-1.549441	2.346203
H	-2.692905	-0.829744	-2.828852	H	2.014163	-0.446772	-2.781674
H	-5.104683	-0.873485	-2.188152	H	4.474646	-0.494658	-2.246220
H	-5.753168	-0.827903	0.221666	H	5.220613	-1.227957	0.003999
H	-4.025714	-0.676738	1.975056	H	3.576271	-1.822932	1.761414
H	2.844622	0.526752	-0.959354	H	1.160427	0.858273	2.292659
H	4.674793	-1.021417	-1.572984	H	2.565879	2.837746	1.865127
H	4.855496	-3.243114	-0.455534	H	2.201493	4.221374	-0.174786
H	3.148520	-3.932900	1.218575	H	0.436715	3.556293	-1.808982
H	1.297375	-2.408045	1.808284	H	-0.954446	1.567830	-1.392328
H	2.803370	1.708360	1.948124	H	-2.112169	-2.328417	0.003260
H	3.098255	4.149779	1.619903	H	-4.485318	-2.572771	-0.680493
H	1.594036	5.379390	0.063201	H	-5.950278	-0.565958	-0.842558
H	-0.205161	4.159101	-1.142331	H	-5.023239	1.685295	-0.302346
H	-0.509139	1.715759	-0.784393	H	-2.671279	1.917049	0.412207

S_0-TC				S_0-TT			
C	-0.005772	-0.039803	0.002030	C	-0.004915	-0.010387	0.005194
C	-0.013711	-0.037415	1.392175	C	-0.011639	-0.014356	1.395112
C	1.184459	0.014472	2.099218	C	1.188284	-0.003936	2.102223
C	2.391512	0.065939	1.405030	C	2.395814	0.010191	1.408532
C	2.400424	0.069648	0.016177	C	2.403013	0.021506	0.018478
C	1.200985	0.021385	-0.711035	C	1.203046	0.019304	-0.706720
C	1.202721	0.049028	-2.191146	C	1.203137	0.058529	-2.188395
C	2.209045	0.670972	-2.865020	C	2.151275	0.772445	-2.852453
C	2.375383	0.629559	-4.288868	C	2.338627	0.775727	-4.276124
C	3.313680	1.287816	-5.039233	C	3.185454	1.573846	-4.988085
C	4.326416	2.217395	-4.451142	C	3.234494	1.344744	-6.468472
O	4.396613	2.469925	-3.254803	O	2.552732	0.493435	-7.016656
C	0.068723	-0.610493	-2.887985	C	0.132239	-0.690681	-2.889785
C	-0.255418	-1.944644	-2.606427	C	-0.141058	-2.020597	-2.539464
C	-1.306838	-2.572519	-3.263205	C	-1.131006	-2.738071	-3.199006
C	-2.065668	-1.872739	-4.200196	C	-1.878661	-2.134212	-4.208742
C	-1.764702	-0.542575	-4.476303	C	-1.630000	-0.809369	-4.553122
C	-0.704510	0.083579	-3.826221	C	-0.632519	-0.092652	-3.898883
C	5.260634	2.830524	-5.402626	C	4.153487	2.206477	-7.224159
C	5.206324	2.573914	-6.727257	C	4.897580	3.150687	-6.611311
C	4.223269	1.672627	-7.284709	C	4.830607	3.366233	-5.180057
C	3.329552	1.067420	-6.472554	C	4.013990	2.612701	-4.411904
H	-0.950205	-0.074196	-0.542820	H	-0.948698	-0.017013	-0.542341
H	-0.964624	-0.074835	1.927583	H	-0.962773	-0.025771	1.931292
H	1.178722	0.010415	3.191344	H	1.182428	-0.014718	3.194256
H	3.336561	0.096830	1.950956	H	3.341371	0.001419	1.954566
H	3.352072	0.091062	-0.516481	H	3.353695	0.003216	-0.517283
H	2.962500	1.230286	-2.314385	H	2.836801	1.371631	-2.250368
H	1.693828	-0.023588	-4.842126	H	1.772779	0.058943	-4.876863
H	0.332568	-2.492498	-1.867531	H	0.440023	-2.494998	-1.746482
H	-1.539106	-3.615871	-3.040267	H	-1.322120	-3.777076	-2.923233
H	-2.896890	-2.364430	-4.709571	H	-2.659449	-2.697339	-4.723944
H	-2.362288	0.016433	-5.199352	H	-2.216629	-0.326236	-5.336828
H	-0.478922	1.131477	-4.032144	H	-0.452177	0.950853	-4.160993
H	5.997862	3.508139	-4.968476	H	4.195210	2.036453	-8.301461
H	5.919178	3.054331	-7.402744	H	5.572261	3.777931	-7.200049
H	4.214079	1.488588	-8.360316	H	5.447131	4.147892	-4.732781
H	2.582457	0.383955	-6.884709	H	3.966401	2.790545	-3.336051

Table S6 Cartesian coordinates (in Å) for geometries optimized in Table S1 at CAM-B3LYP-D3/def2-SV(P) level of theory.

S_0-C				S_0-T			
C	1.538194	1.984116	0.958386	C	0.009444	2.181736	1.110396
C	1.781901	3.345220	0.819896	C	0.050901	3.553111	0.852113
C	1.113999	4.079924	-0.160154	C	-0.235616	4.033252	-0.420493
C	0.208567	3.438213	-0.997908	C	-0.566969	3.136783	-1.438125
C	-0.033358	2.070867	-0.859954	C	-0.614907	1.773913	-1.176468
C	0.625939	1.333013	0.120959	C	-0.328444	1.283610	0.102031
C	0.360355	-0.163094	0.304558	C	-0.389587	-0.232293	0.319750
C	-0.163433	-0.377640	1.710967	C	0.062821	-0.645443	1.706122
C	-1.465292	-0.526865	1.961101	C	1.339695	-0.963480	1.934306
C	-2.429205	-0.557707	0.867716	C	2.302180	-0.947151	0.837541
C	-1.918116	-0.599701	-0.436881	C	1.783587	-0.876567	-0.464417
O	-0.585741	-0.607034	-0.678179	O	0.443908	-0.847818	-0.671681
C	1.608225	-1.004601	0.034971	C	-1.801882	-0.760223	0.077600
C	2.593950	-0.572115	-0.853469	C	-2.900633	-0.080144	0.608192
C	3.687651	-1.382934	-1.146698	C	-4.188164	-0.583166	0.447608
C	3.808567	-2.637600	-0.554428	C	-4.392920	-1.770957	-0.251909
C	2.824857	-3.079973	0.327195	C	-3.300920	-2.450538	-0.784321
C	1.731330	-2.268173	0.615509	C	-2.010728	-1.950719	-0.617299
C	-2.774507	-0.684172	-1.531918	C	2.626557	-0.907306	-1.570539
C	-4.151120	-0.708399	-1.328808	C	4.002761	-0.995381	-1.380893
C	-4.677603	-0.654231	-0.037800	C	4.537741	-1.057635	-0.093643
C	-3.813799	-0.585285	1.050054	C	3.685863	-1.038868	1.005665
H	2.078796	1.416710	1.720614	H	0.252306	1.811773	2.108101
H	2.501442	3.837365	1.479720	H	0.316840	4.246866	1.654127
H	1.305360	5.150590	-0.271008	H	-0.199054	5.106739	-0.624789
H	-0.317191	4.002681	-1.772618	H	-0.791602	3.506504	-2.442064
H	-0.735096	1.572201	-1.528248	H	-0.875805	1.068981	-1.969168
H	0.572274	-0.349685	2.517096	H	-0.687587	-0.656042	2.499729
H	-1.832431	-0.631378	2.985916	H	1.682836	-1.249868	2.932598
H	2.507235	0.410003	-1.321834	H	-2.749400	0.860883	1.143042
H	4.452201	-1.030026	-1.844051	H	-5.038655	-0.038345	0.865631
H	4.669114	-3.272593	-0.781635	H	-5.404273	-2.164436	-0.383610
H	2.906880	-4.065733	0.792397	H	-3.451530	-3.382993	-1.334855
H	0.954325	-2.625117	1.296009	H	-1.153074	-2.480806	-1.031519
H	-2.339724	-0.732278	-2.532395	H	2.185066	-0.858384	-2.567691
H	-4.820424	-0.769217	-2.191024	H	4.665574	-1.012155	-2.250037
H	-5.758743	-0.671753	0.118987	H	5.618640	-1.125925	0.051038
H	-4.211198	-0.554977	2.068763	H	4.092444	-1.100445	2.019298

S_0-CC-C				S_0-CC-T			
C	0.344599	1.747077	-0.981340	C	-0.004459	0.012694	0.009072
C	0.961623	2.934352	-0.600788	C	-0.012570	0.011072	1.399896
C	0.834767	3.397942	0.707009	C	1.187701	0.007782	2.107774
C	0.075992	2.675482	1.626370	C	2.396369	0.004155	1.414439
C	-0.543919	1.492670	1.243448	C	2.404002	0.011587	0.023564
C	-0.404568	1.004749	-0.062556	C	1.204260	0.024545	-0.701272
C	-1.034461	-0.275156	-0.451221	C	1.213509	0.052268	-2.183322
C	-0.379443	-1.234551	-1.152192	C	2.146453	0.789957	-2.836197
C	1.013668	-1.309166	-1.536974	C	2.401188	0.908301	-4.255992
C	2.177773	-1.054803	-0.864924	C	2.472716	-0.012335	-5.265294
C	2.249953	-0.743029	0.595588	C	2.426886	-1.491653	-5.053761
O	1.266727	-0.700397	1.319138	O	2.324234	-2.006280	-3.950679
C	-2.462432	-0.466026	-0.102132	C	0.144615	-0.690393	-2.884990
C	-3.359345	0.611098	-0.135658	C	-0.143036	-2.015975	-2.533593
C	-4.703645	0.427661	0.170241	C	-1.120217	-2.731946	-3.213929
C	-5.174890	-0.833682	0.529594	C	-1.835302	-2.131289	-4.248818
C	-4.291480	-1.910097	0.581102	C	-1.574062	-0.806386	-4.591687
C	-2.948385	-1.727471	0.268594	C	-0.592368	-0.092133	-3.912281
C	3.594057	-0.515870	1.141716	C	2.545701	-2.320416	-6.260230
C	4.704475	-0.611501	0.380009	C	2.711355	-1.783247	-7.487635
C	4.627977	-0.961036	-1.021813	C	2.797816	-0.351620	-7.677022
C	3.426550	-1.180146	-1.598605	C	2.694716	0.477337	-6.615886
H	0.436912	1.390059	-2.009161	H	-0.948413	0.016211	-0.540379
H	1.539551	3.505098	-1.332373	H	-0.965191	0.012270	1.936131
H	1.320070	4.329985	1.008287	H	1.181091	-0.000700	3.201166
H	-0.028095	3.033956	2.653675	H	3.342475	-0.016816	1.961683
H	-1.119005	0.915341	1.969454	H	3.353043	-0.023774	-0.516279
H	-0.993852	-2.037059	-1.576826	H	2.748315	1.472508	-2.225093
H	1.154837	-1.700937	-2.554158	H	2.638678	1.936574	-4.563960
H	-2.995644	1.601664	-0.416617	H	0.432654	-2.493331	-1.738774
H	-5.389420	1.277998	0.128460	H	-1.321204	-3.770559	-2.939354
H	-6.229652	-0.976060	0.779208	H	-2.604722	-2.694770	-4.783399
H	-4.648882	-2.898873	0.880203	H	-2.142999	-0.323062	-5.390192
H	-2.253504	-2.567119	0.341753	H	-0.395500	0.949219	-4.174976
H	3.631962	-0.261226	2.203044	H	2.486773	-3.398697	-6.095661
H	5.688617	-0.430077	0.822579	H	2.790835	-2.434150	-8.363679
H	5.549121	-1.047768	-1.602649	H	2.950403	0.047047	-8.682551
H	3.364147	-1.446880	-2.657858	H	2.761077	1.560784	-6.754785

S_1-C				S_1-T			
C	1.587295	2.070954	0.307984	C	0.006594	-0.188418	-0.053410
C	1.590328	3.450012	0.151500	C	0.028107	-0.217647	1.335707
C	0.417801	4.131347	-0.185102	C	1.220470	-0.004890	2.027613
C	-0.758508	3.406134	-0.361214	C	2.392190	0.235501	1.312023
C	-0.775053	2.024877	-0.198868	C	2.376113	0.273159	-0.079114
C	0.403858	1.333612	0.128826	C	1.180447	0.069143	-0.773434
C	0.404977	-0.186712	0.374349	C	1.115132	0.146850	-2.300750
C	-0.137852	-0.340393	1.738035	C	0.571209	1.484210	-2.617921
C	-1.503332	-0.494886	1.944222	C	1.276830	2.404930	-3.380204
C	-2.358403	-0.764143	0.857178	C	2.551086	2.091973	-3.893003
C	-1.764877	-0.886880	-0.469971	C	3.115423	0.790361	-3.559667
O	-0.462500	-0.771136	-0.643266	O	2.461033	-0.057428	-2.782694
C	1.758864	-0.827804	0.108908	C	0.369395	-1.051005	-2.906381
C	2.305321	-0.719750	-1.173136	C	0.636073	-2.337390	-2.426195
C	3.530187	-1.304155	-1.470028	C	-0.001704	-3.439237	-2.983035
C	4.227398	-2.004555	-0.484977	C	-0.911314	-3.268903	-4.027024
C	3.684690	-2.122126	0.789942	C	-1.177345	-1.989092	-4.507760
C	2.450238	-1.542097	1.083650	C	-0.541208	-0.882861	-3.947823
C	-2.543707	-1.153238	-1.607603	C	4.373020	0.377612	-4.019760
C	-3.910558	-1.334026	-1.481472	C	5.137767	1.234641	-4.802799
C	-4.509850	-1.219035	-0.201553	C	4.616768	2.509724	-5.130312
C	-3.760471	-0.938536	0.928008	C	3.365418	2.926228	-4.693246
H	2.514065	1.556137	0.566340	H	-0.927884	-0.375234	-0.588032
H	2.524646	4.001015	0.290599	H	-0.896077	-0.418977	1.884379
H	0.422808	5.217375	-0.306769	H	1.237328	-0.035624	3.119849
H	-1.685133	3.921391	-0.628990	H	3.336041	0.389235	1.842082
H	-1.717510	1.493624	-0.344852	H	3.302815	0.450993	-0.627470
H	0.541289	-0.135620	2.565202	H	-0.385440	1.735868	-2.159790
H	-1.924846	-0.430556	2.949636	H	0.856933	3.394739	-3.572062
H	1.759646	-0.165805	-1.940146	H	1.350257	-2.470041	-1.610418
H	3.946924	-1.211797	-2.476437	H	0.212633	-4.440612	-2.599616
H	5.193889	-2.460211	-0.715456	H	-1.415678	-4.135634	-4.462051
H	4.220604	-2.674023	1.566578	H	-1.891158	-1.847412	-5.323653
H	2.020062	-1.658833	2.079270	H	-0.752465	0.125417	-4.311634
H	-2.031383	-1.219501	-2.569343	H	4.718204	-0.618238	-3.734099
H	-4.522514	-1.556061	-2.357733	H	6.123723	0.931266	-5.158642
H	-5.590199	-1.356451	-0.105701	H	5.216090	3.185597	-5.746185
H	-4.246468	-0.854489	1.902993	H	2.991817	3.916371	-4.964763

CI-S_1/S_0-C				CI-S_1/S_0-T			
C	-1.936154	-0.687134	-0.802375	C	1.410845	-1.235039	-0.857083
C	-2.349720	-0.631696	0.610768	C	1.869632	-1.525554	0.491929
C	-1.440626	-0.510581	1.710700	C	0.837142	-1.796481	1.508946
C	-0.110208	-0.252274	1.825795	C	-0.360207	-1.182727	1.584255
C	0.944574	0.110339	0.876068	C	-0.853656	-0.085992	0.741802
O	-0.755073	-0.650897	-1.151887	O	0.217158	-1.417191	-1.169877
C	-3.014260	-0.777961	-1.787518	C	2.385251	-0.738489	-1.797277
C	-4.322105	-0.814060	-1.427981	C	3.729440	-0.760986	-1.492938
C	-4.695645	-0.782953	-0.048669	C	4.152775	-1.175694	-0.219977
C	-3.729593	-0.703279	0.923123	C	3.222846	-1.529297	0.768424
C	1.113188	1.559219	0.612917	C	-2.222255	-0.192396	0.263459
C	1.955399	-0.807058	0.495914	C	-0.044028	1.082966	0.511446
C	2.927001	-0.445573	-0.473558	C	0.997231	1.447305	1.392671
C	3.943581	-1.316501	-0.816439	C	1.785408	2.566031	1.151497
C	4.037743	-2.568014	-0.199123	C	1.581193	3.340073	0.012138
C	3.078894	-2.953902	0.740298	C	0.580177	2.979267	-0.893661
C	2.041215	-2.100083	1.072238	C	-0.217267	1.874369	-0.652255
C	2.138662	2.252412	1.273591	C	-2.764982	-1.457636	-0.038234
C	2.304895	3.620181	1.086949	C	-4.088242	-1.584666	-0.439474
C	1.460912	4.308007	0.219210	C	-4.905059	-0.458814	-0.539065
C	0.447305	3.625544	-0.448537	C	-4.385419	0.800526	-0.242880
C	0.262038	2.262273	-0.245211	C	-3.060227	0.933959	0.149963
H	-1.944052	-0.615704	2.677396	H	1.071563	-2.544078	2.274590
H	0.243314	-0.219302	2.867972	H	-1.056213	-1.549441	2.346203
H	-2.692905	-0.829744	-2.828852	H	2.014163	-0.446772	-2.781674
H	-5.104683	-0.873485	-2.188152	H	4.474646	-0.494658	-2.246220
H	-5.753168	-0.827903	0.221666	H	5.220613	-1.227957	0.003999
H	-4.025714	-0.676738	1.975056	H	3.576271	-1.822932	1.761414
H	2.844622	0.526752	-0.959354	H	1.160427	0.858273	2.292659
H	4.674793	-1.021417	-1.572984	H	2.565879	2.837746	1.865127
H	4.855496	-3.243114	-0.455534	H	2.201493	4.221374	-0.174786
H	3.148520	-3.932900	1.218575	H	0.436715	3.556293	-1.808982
H	1.297375	-2.408045	1.808284	H	-0.954446	1.567830	-1.392328
H	2.803370	1.708360	1.948124	H	-2.112169	-2.328417	0.003260
H	3.098255	4.149779	1.619903	H	-4.485318	-2.572771	-0.680493
H	1.594036	5.379390	0.063201	H	-5.950278	-0.565958	-0.842558
H	-0.205161	4.159101	-1.142331	H	-5.023239	1.685295	-0.302346
H	-0.509139	1.715759	-0.784393	H	-2.671279	1.917049	0.412207

S_0-TC				S_0-TT			
C	-0.005366	-0.031201	0.003057	C	-0.004976	-0.009330	0.006781
C	-0.014787	-0.029674	1.393802	C	-0.013145	-0.013974	1.397339
C	1.183849	0.009692	2.102214	C	1.186819	-0.007220	2.105705
C	2.392287	0.049356	1.408526	C	2.395345	0.003867	1.412402
C	2.401904	0.054229	0.018920	C	2.403182	0.016056	0.021683
C	1.202515	0.018589	-0.709629	C	1.203605	0.017415	-0.704783
C	1.204580	0.047564	-2.189924	C	1.204303	0.057708	-2.186519
C	2.211070	0.670765	-2.863445	C	2.153153	0.772416	-2.849844
C	2.379430	0.627992	-4.288288	C	2.342191	0.775567	-4.274412
C	3.314629	1.289760	-5.040166	C	3.187017	1.575109	-4.988139
C	4.320886	2.227933	-4.454568	C	3.235777	1.342633	-6.468124
O	4.387646	2.485938	-3.259445	O	2.555399	0.488855	-7.014070
C	0.070617	-0.611094	-2.887327	C	0.133622	-0.690506	-2.889176
C	-0.261747	-1.941887	-2.598146	C	-0.144440	-2.019074	-2.536388
C	-1.313726	-2.569789	-3.255376	C	-1.134664	-2.736362	-3.197093
C	-2.065514	-1.872452	-4.200806	C	-1.878311	-2.132891	-4.210929
C	-1.756762	-0.544949	-4.484493	C	-1.625209	-0.808835	-4.557824
C	-0.695731	0.080305	-3.833646	C	-0.627194	-0.093078	-3.902032
C	5.253015	2.842964	-5.407277	C	4.151623	2.205247	-7.226803
C	5.202074	2.581107	-6.731784	C	4.894335	3.153508	-6.616800
C	4.224572	1.671519	-7.287032	C	4.827929	3.372026	-5.185494
C	3.333145	1.063870	-6.472961	C	4.013411	2.617483	-4.414752
H	-0.950778	-0.055788	-0.542811	H	-0.949521	-0.012940	-0.541581
H	-0.967654	-0.057961	1.928704	H	-0.965886	-0.023102	1.933102
H	1.177264	0.004887	3.195566	H	1.180184	-0.018574	3.198964
H	3.338438	0.070126	1.955361	H	3.341717	-0.007776	1.959316
H	3.355577	0.065238	-0.512501	H	3.355493	-0.004887	-0.513244
H	2.963516	1.231614	-2.311324	H	2.839071	1.372821	-2.247135
H	1.701379	-0.031821	-4.840189	H	1.777736	0.055238	-4.873748
H	0.320748	-2.488431	-1.852462	H	0.433712	-2.493798	-1.740048
H	-1.551976	-3.611589	-3.025980	H	-1.329082	-3.775319	-2.918877
H	-2.897889	-2.364057	-4.710928	H	-2.659907	-2.695930	-4.727528
H	-2.349089	0.013001	-5.214427	H	-2.208851	-0.325288	-5.345124
H	-0.464481	1.126781	-4.045844	H	-0.443855	0.950415	-4.166446
H	5.986150	3.527210	-4.974181	H	4.192520	2.032640	-8.304702
H	5.913418	3.063472	-7.409344	H	5.567506	3.782083	-7.207982
H	4.217767	1.483216	-8.363149	H	5.443388	4.157104	-4.739855
H	2.589936	0.373680	-6.883834	H	3.966240	2.797990	-3.338201