Supporting Information

Catalyzed *E*/*Z* isomerization mechanism of stilbene using *para*-benzoquinone as a triplet sensitizer

Kaho Nakatani,[1] Hirofumi Sato,[1] Ryoichi Fukuda[1,2,*]

[1]Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Kyoto-Daigaku-Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

[2]Center for the Promotion of Interdisciplinary Education and Research, Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, 1-30 Goryo-Ohara, Nishikyo-ku, Kyoto 615-8245, Japan

CONTENTS

Table S1. Absolute energy values of the considered systems (in Hartree): the total energy (E_{tot}), zero-point energy (ZPE), solvation energy (ΔE_{solv}), and their sum.

	System	E_{tot}	ZPE	ΔE_{solv}	E_{tot} + ZPE + ΔE_{solv}
1	PBQ (S_0 state)	-381.561791	0.084550	-0.004356	-381.481597
2	PBQ (T1 state)	-381.488777	0.081675	-0.004419	-381.411521
3	PBQ (anion doublet state)	-381.641648	0.082785	-0.046629	-381.605492
4	Stilbene (S_0, (*E*)-form)	-540.846680	0.213896	-0.002502	-540.635286
5	Stilbene (S_0, (*Z*)-form)	-540.839204	0.214117	-0.002031	-540.627118
6	Stilbene (S_0, (*tw*)-form)[a]	-540.793127	0.213181	-0.002134	-540.582080
7	Stilbene (T_1, (*E*)-form)[b]	-540.769533	0.210292	-0.002417	-540.561658
8	Stilbene (T_1, (*Z*)-form)[c]	-540.757904	0.210573	-0.001988	-540.549319
9	Stilbene (T_1, (*tw*)-form)	-540.774086	0.210138	-0.002036	-540.565984
10	Stilbene (cation doublet, (*E*)-form)	-540.580033	0.214480	-0.035838	-540.401391
11	Stilbene (cation doublet, (*Z*)-form)	-540.568017	0.214537	-0.035897	-540.389377
12	Stilbene (cation doublet, (*tw*)-form)[a]	-540.542088	0.213077	-0.036200	-540.365211
13	(*E*)-form encounter complex (S_0)	-922.411590	0.299040	-0.005481	-922.118031
14	(*Z*)-form encounter complex (S_0)	-922.403502	0.299360	-0.005314	-922.109456
15	(*E*)-form encounter complex (T_1)	-922.347668	0.297802	-0.009783	-922.059649
16	(*Z*)-form encounter complex (T_1)	-922.339233	0.297963	-0.009034	-922.050304
17	***E*-XP** (T_1)	-922.367493	0.299957	-0.006533	-922.074069
18	***Z*-XP** (T_1)	-922.364099	0.299983	-0.006448	-922.070564
19	***tw*-XP** (T_1)	-922.367224	0.299857	-0.006601	-922.073968
20	**TS1** (T_1)	-922.345246	0.297762	-0.010130	-922.057614
21	**TS2** (T_1)	-922.339010	0.298003	-0.009156	-922.050163
22	**TS3** (T_1)	-922.359142	0.300048	-0.006415	-922.065509
23	**TS4** (T_1)	-922.363984	0.299630	-0.006840	-922.071194
24	**TS5** (T_1)	-922.359884	0.299691	-0.006379	-922.066572
25	**CP1** (S_0)	-922.345967	0.298465	-0.007213	-922.054715
26	**CP1** (T_1)	-922.345967	0.297289	-0.007455	-922.056133
27	**CP2** (S_0)	-922.339819	0.299732	-0.007620	-922.047707
28	**CP2** (T_1)	-922.339820	0.299107	-0.006119	-922.046832
29	***E*-OX** (S_0)	-922.386483	0.303382	-0.006117	-922.089218
30	***E*-OX** (T_1)	-922.293345	0.299671	-0.004384	-921.998058
31	***Z*-OX** (S_0)	-922.381624	0.303508	-0.005908	-922.084024
32	***Z*-OX** (T_1)	-922.288656	0.299963	-0.004127	-921.992820
33	Diacetyl (S_0 state)	-306.571692	0.092618	-0.003400	-306.482474
34	Diacetyl (T_1 state)	-306.495909	0.090904	-0.002537	-306.407542
35	Diacetyl (anion doublet state)	-306.607756	0.090749	-0.050026	-306.567033
36	(*E*)-form encounter complex with diacetyl (T_1)	-847.345064	0.305263	-0.003981	-847.043782
37	**TS**: (*E*)-form with diacetyl (T_1)	-847.330445	0.305676	-0.007341	-847.032110
38	Exciplex: (*E*)-form with diacetyl (T_1)	-847.348632	0.308244	-0.005857	-847.046245
39	Oxetane: (*E*)-form with diacetyl (T_1)	-847.284242	0.309293	-0.003742	-846.978691

[a] The maximum energy structure with respective to the central-bond torsion; other coordinates was relaxed.

[b]Involving one imaginary frequency mode with $18.2i$ cm^{-1}.

[c]The dihedral angle for the central-bond torsion was fixed at the S_0 state value of (*Z*)-form.

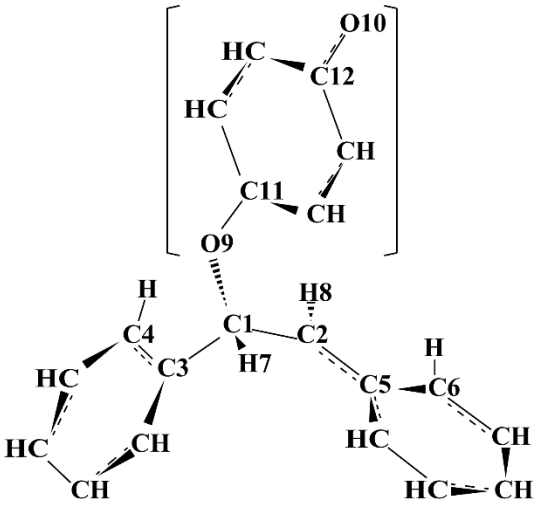


Figure S1. Numberings of atoms used in Table S2.

Table S2. Selected structural parameters of relevant compounds.

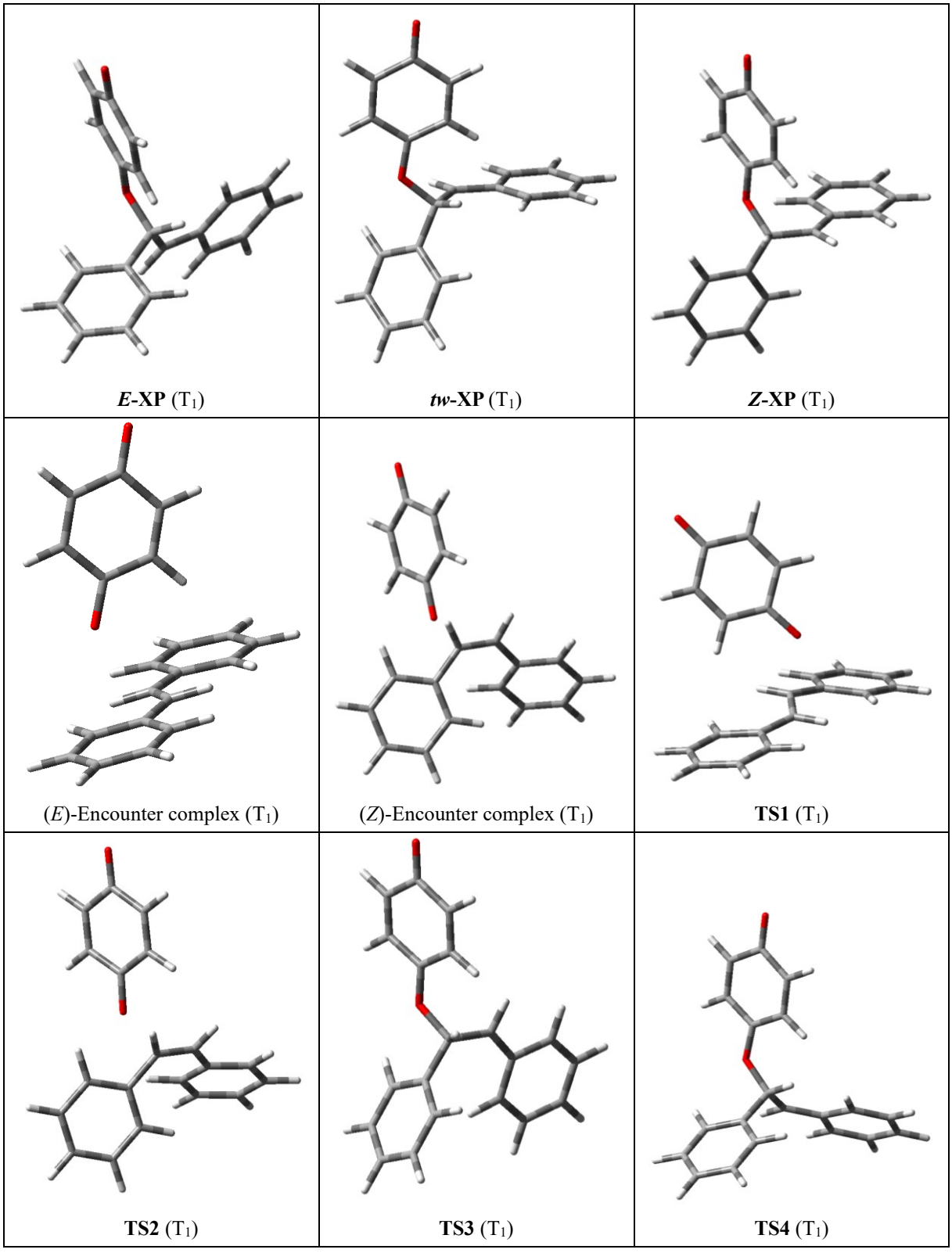
	Bond length / Å				Dihedral angle / degree	
System (state)	C1C2	C1C3	C2C5	C1O9	C3C1C2C5	C2C1O9C11
(*E*)-Stilbene (S_0)	1.345	1.466	1.466		180.0	
(*tw*)-Stilbene (S_0)	1.382	1.466	1.466		92.0	
(*Z*)-Stilbene (S_0)	1.346	1.475	1.475		6.4	
(*E*)-Stilbene (T_1)	1.462	1.395	1.395		180.0[a]	
(*tw*)-Stilbene (T_1)	1.466	1.416	1.416		90.6	
(*Z*)-Stilbene (T_1)	1.474	1.403	1.403		6.4[b]	
(*E*)-Stilbene (cation)	1.387	1.424	1.424		180.0	
(*tw*)-Stilbene (cation)	1.422	1.412	1.412		93.0	
(*Z*)-Stilbene (cation)	1.392	1.427	1.427		23.8	
***E*-XP** (T_1)	1.496	1.518	1.414	1.466	−152.9	−160.3
***tw*-XP** (T_1)	1.497	1.519	1.413	1.456	−103.8	−75.1
***Z*-XP** (T_1)	1.500	1.527	1.414	1.464	78.6	−73.2
(*E*)-Encounter complex (T_1)	1.370	1.446	1.454	2.800	−174.9	−111.3
(*Z*)-Encounter complex (T_1)	1.376	1.462	1.452	2.400	17.2	−92.5
TS1 (T_1)	1.394	1.459	1.438	2.114	−162.2	−110.8
TS2 (T_1)	1.389	1.469	1.445	2.197	26.4	−88.2
TS3 (T_1)	1.503	1.515	1.416	1.469	5.6	−81.7
TS4 (T_1)	1.494	1.520	1.412	1.463	−115.1	−120.6
TS5 (T_1)	1.501	1.523	1.414	1.456	143.7	−120.0
CP1 (S_0)	1.458	1.471	1.412	1.716	−162.6	92.1
CP2 (S_0)	1.482	1.507	1.404	1.572	63.9	70.0
***E*-OX** (T_1)	1.548	1.506	1.503	1.448	109.1	9.0
***E*-OX** (S_0)	1.552	1.505	1.503	1.451	107.4	10.8
***Z*-OX** (T_1)	1.533	1.509	1.504	1.445	6.3	−1.6
***Z*-OX** (S_0)	1.568	1.506	1.505	1.447	−1.0	4.2

[a]One imaginary frequency mode is involved. [b]Fixed dihedral angle.

Table S3. Relative energies (kcal mol^{-1}) calculated with B3LYP, wB97XD and M06-2x.

System (state)	B3LYP	ωB97XD	M06-2x
(*E*)-Stilbene (S_0) + PBQ (T_1)	0.0	0.0	0.0
(*E*)-Encounter complex (T_1)	−8.1	−9.0	−7.5
TS1 (T_1)	−6.8	−8.9	−6.9
***E*-XP** (T_1)	−17.1	−28.3	−28.9

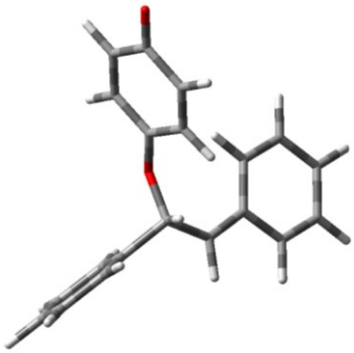
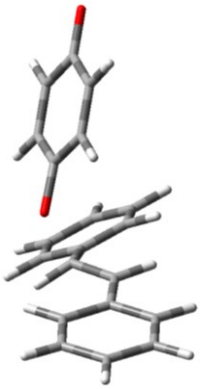
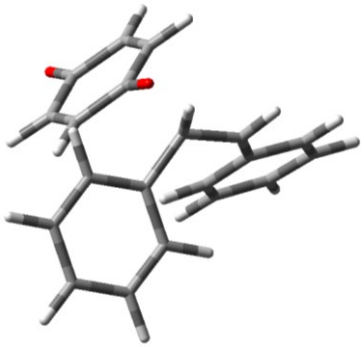
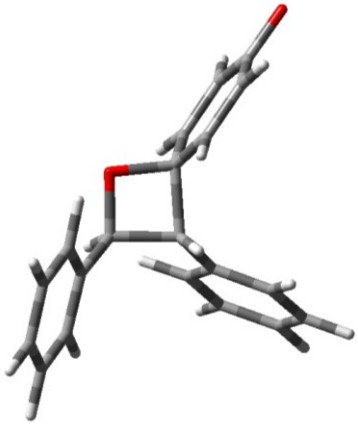
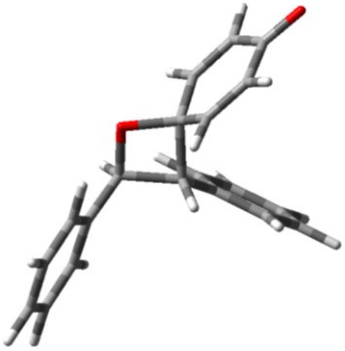
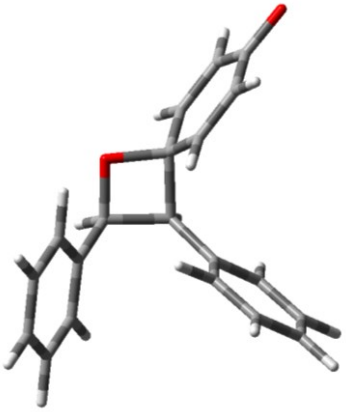
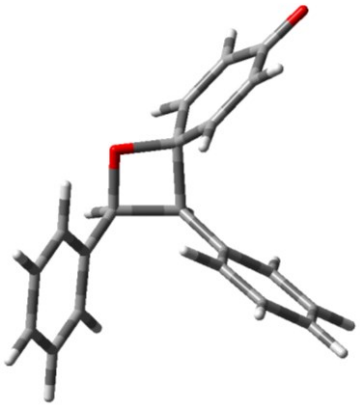
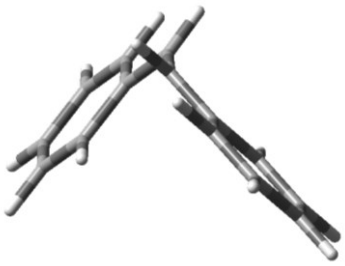
Figure S2. Three dimensional structures of the intermediate species.



***E*-XP** (T_1) | ***tw*-XP** (T_1) | ***Z*-XP** (T_1)

(*E*)-Encounter complex (T_1) | (*Z*)-Encounter complex (T_1) | **TS1** (T_1)

TS2 (T_1) | **TS3** (T_1) | **TS4** (T_1)

 **TS5** (T_1)	 **CP1** (S_0)	 **CP2** (S_0)
 ***E*-OX** (T_1)	 ***E*-OX** (S_0)	 ***Z*-OX** (T_1)
 ***Z*-OX** (S_0)	 (*tw*)-Stilbene (T_1)	

Cartesian Coordinates (in Å)

1. PBQ (S0 state)

	X	Y	Z
O	0.000000	-0.000000	2.662245
O	0.000000	-0.000000	-2.662245
C	0.000000	-0.000000	1.442568
C	0.000000	1.269007	0.669693
C	-0.000000	-1.269007	0.669693
C	0.000000	1.269007	-0.669693
C	-0.000000	-1.269007	-0.669693
C	0.000000	-0.000000	-1.442568
H	0.000000	2.181751	1.255199
H	-0.000000	-2.181751	1.255199
H	0.000000	2.181751	-1.255199
H	-0.000000	-2.181751	-1.255199

2. PBQ (T1 state)

	X	Y	Z
O	0.000000	-0.000000	2.698930
O	0.000000	0.000000	-2.694229
C	0.000000	-0.000000	1.398614
C	0.000000	1.241450	0.691180
C	-0.000000	-1.241450	0.691180
C	0.000000	1.231022	-0.676217
C	-0.000000	-1.231022	-0.676217
C	0.000000	0.000000	-1.444991
H	0.000000	2.160841	1.262162
H	-0.000000	-2.160841	1.262162
H	0.000000	2.162165	-1.231613
H	-0.000000	-2.162165	-1.231613

3. PBQ (anion doublet state)

	X	Y	Z
O	0.000000	0.000000	2.732766
O	0.000000	-0.000000	-2.732657
C	0.000000	0.000000	1.466139
C	-0.000000	1.221371	0.685347
C	-0.000000	-1.221371	0.685347
C	-0.000000	1.222062	-0.685266
C	-0.000000	-1.222062	-0.685266
C	0.000000	-0.000000	-1.466379
H	-0.000000	2.153461	1.245337
H	-0.000000	-2.153461	1.245337
H	-0.000000	2.153870	-1.245538
H	-0.000000	-2.153870	-1.245538

4. Stilbene (S0, (E)-form)

	X	Y	Z
C	-0.497168	-0.453238	-0.000083
C	0.497159	0.453196	0.000032
H	-0.241248	-1.509580	-0.000239
H	0.241247	1.509539	0.000148
C	-1.938449	-0.186191	-0.000039
C	-2.491330	1.107820	0.000093
C	-2.826600	-1.275566	-0.000138
C	-3.867275	1.297401	0.000123
H	-1.841638	1.975037	0.000161
C	-4.205732	-1.086565	-0.000097
H	-2.424186	-2.283506	-0.000240
C	-4.734142	0.202140	0.000036
H	-4.268791	2.304811	0.000226
H	-4.866820	-1.946112	-0.000180
H	-5.807354	0.354568	0.000062

C	1.938439	0.186163	0.000031
C	2.826569	1.275553	-0.000108
C	2.491357	-1.107833	0.000173
C	4.205712	1.086590	-0.000137
H	2.424142	2.283488	-0.000197
C	3.867302	-1.297378	0.000136
H	1.841700	-1.975079	0.000328
C	4.734153	-0.202097	-0.000024
H	4.866762	1.946167	-0.000256
H	4.268846	-2.304778	0.000247
H	5.807365	-0.354521	-0.000055

5. Stilbene (S0, (Z)-form)

	X	Y	Z
C	-0.672985	1.848702	0.006019
C	0.672923	1.848613	-0.006008
H	-1.145190	2.828313	-0.028937
H	1.145232	2.828198	0.028800
C	-1.631352	0.729368	0.077291
C	-1.399210	-0.425533	0.841729
C	-2.863190	0.845117	-0.587223
C	-2.352937	-1.435656	0.913992
H	-0.471520	-0.524138	1.391493
C	-3.813448	-0.170552	-0.524466
H	-3.071196	1.740376	-1.164443
C	-3.560926	-1.317849	0.225392
H	-2.156268	-2.315520	1.516725
H	-4.753032	-0.062637	-1.055004
H	-4.301861	-2.107201	0.283016
C	1.631295	0.729281	-0.077279
C	2.863191	0.845175	0.587102
C	1.399155	-0.425699	-0.841595
C	3.813512	-0.170435	0.524339
H	3.071196	1.740501	1.164216
C	2.352947	-1.435762	-0.913866
H	0.471410	-0.524432	-1.391245
C	3.560999	-1.317811	-0.225402
H	4.753138	-0.062403	1.054777
H	2.156273	-2.315691	-1.516503
H	4.301988	-2.107110	-0.283043

6. Stilbene (S0, (tw)-form)

	X	Y	Z
C	-0.599962	-1.224253	0.342387
C	0.599962	-1.224253	-0.342388
H	-0.900236	-2.258512	0.536841
H	0.900237	-2.258512	-0.536842
C	-1.842294	-0.470049	0.152137
C	-1.891206	0.747084	-0.557790
C	-3.048843	-0.984519	0.660930
C	-3.097667	1.399848	-0.772114
H	-0.975904	1.158326	-0.968793
C	-4.255523	-0.326260	0.449243
H	-3.033607	-1.917713	1.214527
C	-4.287826	0.868773	-0.268404
H	-3.114737	2.324844	-1.338091
H	-5.173572	-0.748512	0.842658
H	-5.229183	1.377823	-0.440635
C	1.842294	-0.470049	-0.152138
C	3.048843	-0.984519	-0.660930
C	1.891206	0.747085	0.557789
C	4.255523	-0.326260	-0.449242
H	3.033607	-1.917713	-1.214527
C	3.097667	1.399848	0.772114
H	0.975904	1.158326	0.968792

C	4.287826	0.868773	0.268405
H	5.173572	-0.748512	-0.842657
H	3.114736	2.324844	1.338091
H	5.229183	1.377823	0.440636

7. Stilbene (T1, (E)-form)

	X	Y	Z
C	0.535465	0.497530	-0.000062
C	-0.535465	-0.497530	-0.000059
H	0.251870	1.543526	-0.000104
H	-0.251870	-1.543526	-0.000091
C	1.903076	0.221470	-0.000024
C	2.448486	-1.109687	0.000038
C	2.850778	1.304153	-0.000046
C	3.813543	-1.319927	0.000074
H	1.782539	-1.962647	0.000060
C	4.206791	1.074469	-0.000010
H	2.471421	2.320727	-0.000093
C	4.709824	-0.241525	0.000051
H	4.196776	-2.334658	0.000122
H	4.894944	1.912679	-0.000029
H	5.778725	-0.418064	0.000078
C	-1.903076	-0.221470	-0.000027
C	-2.850778	-1.304153	-0.000042
C	-2.448486	1.109687	0.000023
C	-4.206791	-1.074469	-0.000011
H	-2.471421	-2.320727	-0.000079
C	-3.813543	1.319927	0.000054
H	-1.782539	1.962647	0.000039
C	-4.709824	0.241525	0.000037
H	-4.894944	-1.912679	-0.000024
H	-4.196776	2.334658	0.000092
H	-5.778725	0.418064	0.000061

8. Stilbene (T1, (Z)-form)

	X	Y	Z
C	-0.056597	0.733697	1.768326
C	0.056597	-0.733697	1.768326
H	0.229018	1.171147	2.724293
H	-0.229018	-1.171147	2.724293
C	-0.186884	1.663480	0.726017
C	-0.754135	1.365970	-0.559452
C	0.175192	3.033277	0.965257
C	-0.874265	2.344446	-1.529402
H	-1.129820	0.371384	-0.754685
C	0.056597	3.992263	-0.015826
H	0.577147	3.297936	1.937592
C	-0.460471	3.659475	-1.281323
H	-1.312011	2.091471	-2.489105
H	0.362498	5.012296	0.189462
H	-0.556136	4.418009	-2.049135
C	0.186884	-1.663480	0.726017
C	-0.175192	-3.033277	0.965257
C	0.754135	-1.365970	-0.559452
C	-0.056597	-3.992263	-0.015826
H	-0.577147	-3.297936	1.937592
C	0.874265	-2.344446	-1.529402
H	1.129820	-0.371384	-0.754685
C	0.460471	-3.659475	-1.281323
H	-0.362498	-5.012296	0.189462
H	1.312011	-2.091471	-2.489105
H	0.556136	-4.418009	-2.049135

9. Stilbene (T1, (tw)-form)

	X	Y	Z
C	0.227553	0.696676	1.394305
C	-0.227553	-0.696676	1.394305
H	0.999172	0.972723	2.113554
H	-0.999172	-0.972723	2.113554
C	-0.295417	1.732943	0.583749
C	-1.312842	1.500315	-0.384714
C	0.190187	3.065802	0.715537
C	-1.806119	2.535583	-1.161238
H	-1.697577	0.494709	-0.509316
C	-0.310710	4.090994	-0.066910
H	0.965433	3.269097	1.447146
C	-1.312842	3.837015	-1.012114
H	-2.581358	2.334393	-1.892642
H	0.075342	5.097380	0.053268
H	-1.702893	4.642269	-1.623694
C	0.295417	-1.732943	0.583749
C	-0.190187	-3.065802	0.715537
C	1.312842	-1.500315	-0.384714
C	0.310710	-4.090994	-0.066910
H	-0.965433	-3.269097	1.447146
C	1.806119	-2.535583	-1.161238
H	1.697577	-0.494709	-0.509316
C	1.312842	-3.837015	-1.012114
H	-0.075342	-5.097380	0.053268
H	2.581358	-2.334393	-1.892642
H	1.702893	-4.642269	-1.623694

10. Stilbene (cation doublet, (E)-form)

	X	Y	Z
C	0.512456	0.467232	-0.000001
C	-0.512456	-0.467232	0.000002
H	0.247089	1.519597	-0.000006
H	-0.247089	-1.519597	0.000006
C	1.908927	0.191062	0.000001
C	2.452636	-1.126204	0.000016
C	2.809190	1.294901	-0.000010
C	3.817759	-1.316959	0.000019
H	1.798813	-1.988849	0.000027
C	4.174710	1.094423	-0.000008
H	2.407068	2.301742	-0.000021
C	4.683946	-0.211310	0.000006
H	4.225399	-2.320266	0.000030
H	4.850913	1.940199	-0.000018
H	5.756042	-0.370312	0.000008
C	-1.908927	-0.191062	-0.000002
C	-2.809190	-1.294901	-0.000006
C	-2.452636	1.126204	0.000001
C	-4.174710	-1.094423	-0.000009
H	-2.407068	-2.301742	-0.000007
C	-3.817759	1.316959	-0.000002
H	-1.798813	1.988849	0.000006
C	-4.683946	0.211310	-0.000007
H	-4.850913	-1.940199	-0.000013
H	-4.225399	2.320266	-0.000000
H	-5.756042	0.370312	-0.000010

11. Stilbene (cation doublet, (Z)-form)

	X	Y	Z
C	0.104574	0.688165	1.735148
C	-0.104574	-0.688165	1.735148
H	0.316483	1.105024	2.717621
H	-0.316483	-1.105024	2.717621
C	0.029351	1.656855	0.690148

C	-0.664271	1.445820	-0.536257
C	0.604786	2.937021	0.931400
C	-0.727493	2.448218	-1.482901
H	-1.185487	0.513212	-0.705819
C	0.560261	3.923288	-0.033484
H	1.102782	3.121522	1.876546
C	-0.104574	3.682275	-1.244011
H	-1.274770	2.290420	-2.404134
H	1.024523	4.884686	0.148020
H	-0.158119	4.464368	-1.992491
C	-0.029351	-1.656855	0.690148
C	-0.604786	-2.937021	0.931400
C	0.664271	-1.445820	-0.536257
C	-0.560261	-3.923288	-0.033484
H	-1.102782	-3.121522	1.876546
C	0.727493	-2.448218	-1.482901
H	1.185487	-0.513212	-0.705819
C	0.104574	-3.682275	-1.244011
H	-1.024523	-4.884686	0.148020
H	1.274770	-2.290420	-2.404134
H	0.158119	-4.464368	-1.992491

12. Stilbene (cation doublet, (tw)-form)

	X	Y	Z
C	-0.610504	0.364756	1.362645
C	0.610501	-0.364769	1.362643
H	-0.536199	1.402760	1.695359
H	0.536196	-1.402776	1.695347
C	-1.759138	0.097548	0.585892
C	-1.911204	-1.097823	-0.176497
C	-2.796863	1.074680	0.542428
C	-3.035475	-1.287391	-0.952133
H	-1.132761	-1.850908	-0.159346
C	-3.912875	0.875086	-0.245199
H	-2.696382	1.978961	1.131966
C	-4.036744	-0.304261	-0.990834
H	-3.146537	-2.192275	-1.536784
H	-4.694110	1.624128	-0.281872
H	-4.914648	-0.459127	-1.607267
C	1.759137	-0.097554	0.585895
C	2.796862	-1.074685	0.542423
C	1.911204	1.097825	-0.176484
C	3.912875	-0.875084	-0.245199
H	2.696380	-1.978971	1.131953
C	3.035476	1.287400	-0.952115
H	1.132761	1.850909	-0.159327
C	4.036746	0.304270	-0.990823
H	4.694111	-1.624125	-0.281877
H	3.146540	2.192289	-1.536758
H	4.914651	0.459142	-1.607253

13. (E)-form encounter complex (S0)

	X	Y	Z
C	2.002334	-1.202321	0.334201
C	1.832846	-0.057723	-0.354675
H	2.733452	-1.228806	1.138459
H	1.101401	-0.032547	-1.157542
C	1.296848	-2.470049	0.121905
C	1.620848	-3.568542	0.937101
C	0.303733	-2.650990	-0.859846
C	0.986442	-4.797933	0.782252
H	2.383658	-3.451929	1.700446
C	-0.328618	-3.878647	-1.013586
H	0.019813	-1.827781	-1.504591
C	0.007579	-4.959839	-0.195564

H	1.257776	-5.628554	1.424413
H	-1.088813	-3.995255	-1.778347
H	-0.488299	-5.915581	-0.321499
C	2.536470	1.211313	-0.143911
C	3.518162	1.407120	0.845136
C	2.217344	2.300628	-0.973523
C	4.147902	2.636361	0.993597
H	3.794814	0.592595	1.504272
C	2.848629	3.532606	-0.825208
H	1.464248	2.170525	-1.743847
C	3.817634	3.707526	0.160089
H	4.901984	2.762413	1.762825
H	2.583992	4.355172	-1.480433
H	4.312120	4.664825	0.279163
C	-2.306483	0.727582	-0.975927
O	-1.481446	0.433727	-1.828235
C	-2.020907	0.554139	0.470371
C	-3.635066	1.272874	-1.352485
C	-2.929319	0.879680	1.400134
C	-4.542487	1.597624	-0.422158
C	-4.258662	1.425102	1.026330
O	-5.086172	1.720243	1.872386
H	-1.044495	0.154726	0.721317
H	-2.745030	0.763465	2.462402
H	-5.519490	1.997505	-0.670409
H	-3.817558	1.388393	-2.415238

14. (Z)-form encounter complex (S0)

	X	Y	Z
C	1.219606	0.748780	-1.575284
C	1.489585	-0.567955	-1.664690
H	0.615453	1.161972	-2.380165
H	1.143909	-1.056993	-2.573380
C	1.624029	1.746598	-0.565389
C	2.904742	1.765103	0.009620
C	0.722439	2.766681	-0.219171
C	3.261519	2.756016	0.918622
H	3.626847	1.007555	-0.269682
C	1.077482	3.750706	0.700370
H	-0.266214	2.775830	-0.666423
C	2.347740	3.748976	1.274226
H	4.258830	2.758716	1.344720
H	0.363077	4.523567	0.961713
H	2.628599	4.520102	1.982794
C	2.167972	-1.481004	-0.725911
C	2.102987	-1.338446	0.670343
C	2.855011	-2.591923	-1.243098
C	2.722813	-2.257549	1.510652
H	1.558369	-0.506564	1.098830
C	3.485142	-3.505746	-0.402929
H	2.898333	-2.732889	-2.318345
C	3.423579	-3.341125	0.979527
H	2.654843	-2.130626	2.585538
H	4.017878	-4.349388	-0.827575
H	3.906993	-4.054507	1.637299
C	-3.237717	0.901871	-0.542997
O	-2.718901	1.897264	-1.024523
C	-2.449516	-0.326063	-0.268880
C	-4.684559	0.875987	-0.209067
C	-3.023097	-1.415529	0.260459
C	-5.257074	-0.213726	0.319425
C	-4.469547	-1.443534	0.594453
O	-4.992841	-2.435205	1.074887
H	-1.395581	-0.285343	-0.522925
H	-2.468349	-2.323529	0.469849
H	-6.310747	-0.258301	0.572202

H	-5.237134	1.785222	-0.419051

15. (E)-form encounter complex (T1)

	X	Y	Z
C	1.439343	1.087948	0.521527
C	0.606691	1.597700	-0.440096
H	1.162076	1.217877	1.563682
H	0.887555	1.486197	-1.479207
C	2.691921	0.397481	0.311916
C	3.457031	0.039353	1.441967
C	3.190788	0.059103	-0.964884
C	4.672858	-0.616201	1.306574
H	3.082595	0.282437	2.430747
C	4.404303	-0.597993	-1.095808
H	2.615443	0.293505	-1.850580
C	5.151979	-0.936386	0.035798
H	5.245534	-0.882048	2.187423
H	4.771193	-0.856544	-2.082383
H	6.099496	-1.451232	-0.074153
C	-0.597642	2.380571	-0.211540
C	-1.039856	2.775479	1.067235
C	-1.361147	2.772642	-1.327661
C	-2.198742	3.523521	1.216784
H	-0.471756	2.506165	1.949567
C	-2.523092	3.519022	-1.175825
H	-1.037650	2.472159	-2.318258
C	-2.947174	3.896752	0.097491
H	-2.522737	3.820328	2.207657
H	-3.099564	3.803879	-2.048242
H	-3.853211	4.478880	0.219725
C	-0.828381	-1.559270	-0.586645
O	0.100410	-0.791153	-1.064739
C	-1.623156	-1.196330	0.544862
C	-1.072339	-2.827732	-1.212682
C	-2.589415	-2.039922	1.021475
C	-2.039020	-3.666897	-0.734261
C	-2.861249	-3.329414	0.414043
O	-3.745968	-4.099988	0.852049
H	-1.439315	-0.234751	1.007248
H	-3.190668	-1.766802	1.881874
H	-2.222731	-4.626536	-1.205238
H	-0.463995	-3.090925	-2.069963

16. (Z)-form encounter complex (T1)

	X	Y	Z
C	0.645267	0.573110	-1.283402
C	0.860546	-0.785109	-1.318831
H	-0.155344	0.928823	-1.924173
H	0.276891	-1.325970	-2.059982
C	1.423316	1.640428	-0.656460
C	2.811519	1.550061	-0.448378
C	0.775511	2.848380	-0.338862
C	3.518717	2.623530	0.079995
H	3.339284	0.646397	-0.724405
C	1.481528	3.912904	0.206748
H	-0.292217	2.933808	-0.503700
C	2.856394	3.803977	0.418804
H	4.590335	2.542390	0.221948
H	0.962492	4.829603	0.461719
H	3.410247	4.637664	0.835196
C	1.710294	-1.632476	-0.501039
C	2.074268	-1.308216	0.822217
C	2.119411	-2.877010	-1.022905
C	2.845591	-2.183736	1.573426
H	1.712726	-0.389551	1.263165

C	2.909166	-3.739967	-0.274735
H	1.818241	-3.155075	-2.027433
C	3.276784	-3.394753	1.026449
H	3.103232	-1.929568	2.595181
H	3.227004	-4.685891	-0.697642
H	3.880997	-4.073200	1.617850
C	-2.194460	0.032876	0.326940
O	-0.918007	0.205604	0.500166
C	-2.769274	-0.394120	-0.909568
C	-3.075273	0.285479	1.432393
C	-4.123215	-0.549431	-1.040619
C	-4.426110	0.129057	1.300820
C	-5.040219	-0.295789	0.055130
O	-6.278296	-0.436082	-0.066444
H	-2.104332	-0.599983	-1.740115
H	-4.558360	-0.875946	-1.978718
H	-5.091085	0.321529	2.135727
H	-2.628253	0.603617	2.366866

17. E-XP (T1)

	X	Y	Z
C	-0.418112	0.556585	0.025993
C	-1.818298	0.650093	-0.492387
H	-0.422717	0.134382	1.035373
H	-2.027908	1.459055	-1.183221
C	0.261844	1.913731	0.055578
C	0.230484	2.677562	1.225488
C	0.872312	2.439679	-1.086166
C	0.799621	3.949147	1.256177
H	-0.242709	2.278438	2.117546
C	1.445077	3.709458	-1.054127
H	0.909354	1.849281	-1.994293
C	1.409258	4.467893	0.115232
H	0.771143	4.530476	2.170827
H	1.922775	4.105651	-1.943138
H	1.857496	5.454591	0.138323
C	-2.868781	-0.237586	-0.163018
C	-2.702034	-1.371218	0.681230
C	-4.170216	-0.006903	-0.694129
C	-3.769525	-2.203035	0.975964
H	-1.726106	-1.601147	1.091124
C	-5.228800	-0.845000	-0.393278
H	-4.322689	0.848306	-1.343841
C	-5.039164	-1.949406	0.445753
H	-3.616291	-3.062427	1.619128
H	-6.209500	-0.644465	-0.809968
H	-5.868939	-2.605743	0.680354
C	1.429044	-0.988826	-0.430024
O	0.291439	-0.387681	-0.841494
C	2.098913	-0.716974	0.783869
C	1.943287	-1.964140	-1.323641
C	3.241999	-1.412194	1.102819
C	3.079795	-2.658110	-1.016532
C	3.797223	-2.423890	0.225184
O	4.836564	-3.056054	0.520500
H	1.732814	0.048129	1.454833
H	3.774172	-1.216683	2.026468
H	3.481549	-3.409286	-1.686453
H	1.399968	-2.139872	-2.245007

18. Z-XP (T1)

	X	Y	Z
C	-0.582796	-0.704667	-0.814156
C	-0.647615	0.715374	-1.293433
H	-0.191047	-1.318269	-1.632869

H	-0.642166	0.839421	-2.371941
C	-1.901846	-1.339386	-0.379404
C	-3.101465	-0.628611	-0.339505
C	-1.906591	-2.699603	-0.045213
C	-4.286644	-1.263912	0.035205
H	-3.115279	0.422117	-0.600338
C	-3.085955	-3.331953	0.332458
H	-0.978990	-3.261021	-0.073360
C	-4.282209	-2.613713	0.373168
H	-5.211562	-0.698961	0.063162
H	-3.074272	-4.384631	0.591787
H	-5.203086	-3.106253	0.664273
C	-0.735414	1.890385	-0.510986
C	-0.803553	1.893762	0.912143
C	-0.765026	3.155159	-1.168530
C	-0.896714	3.084253	1.614013
H	-0.780006	0.954513	1.447387
C	-0.855956	4.336049	-0.454410
H	-0.712804	3.181159	-2.251959
C	-0.922339	4.312006	0.943714
H	-0.948051	3.061609	2.696952
H	-0.874814	5.283603	-0.981131
H	-0.991726	5.237798	1.502764
C	1.665676	-0.837384	0.141396
O	0.328120	-0.881450	0.317826
C	2.316550	-0.586662	-1.087173
C	2.428569	-1.078654	1.313323
C	3.690557	-0.586319	-1.145001
C	3.794419	-1.079662	1.266556
C	4.509448	-0.833978	0.025788
O	5.759797	-0.833833	-0.031102
H	1.743097	-0.380878	-1.980827
H	4.209975	-0.393260	-2.076369
H	4.389786	-1.264754	2.152934
H	1.891043	-1.264831	2.236018

19. tw-XP (T1)

	X	Y	Z
C	-0.511130	-0.589461	-0.153623
C	-0.696693	0.563632	0.783461
H	-0.314640	-0.254247	-1.174791
H	-0.656662	0.306456	1.837592
C	-1.733583	-1.491218	-0.165669
C	-2.622068	-1.443076	-1.242018
C	-2.012181	-2.339522	0.911802
C	-3.774965	-2.226609	-1.243585
H	-2.413832	-0.794631	-2.086766
C	-3.159621	-3.126789	0.906426
H	-1.321003	-2.395804	1.744283
C	-4.046738	-3.069874	-0.168991
H	-4.454689	-2.182618	-2.086996
H	-3.361966	-3.787228	1.742157
H	-4.940686	-3.683037	-0.170371
C	-0.986912	1.901588	0.435916
C	-1.105908	2.367639	-0.905100
C	-1.169020	2.863024	1.472983
C	-1.378420	3.698420	-1.177609
H	-0.988844	1.678431	-1.732710
C	-1.441980	4.188178	1.188110
H	-1.086650	2.536652	2.504096
C	-1.548526	4.620191	-0.139551
H	-1.462858	4.025952	-2.207897
H	-1.573356	4.895859	1.998992
H	-1.762143	5.659030	-0.361396
C	1.881781	-1.016748	0.093266
O	0.605625	-1.418363	0.277149

C	2.271061	0.210214	-0.488182
C	2.864758	-1.944750	0.523929
C	3.607184	0.498679	-0.640818
C	4.194778	-1.666745	0.376946
C	4.646024	-0.421040	-0.219758
O	5.860902	-0.154838	-0.361259
H	1.529857	0.932380	-0.801742
H	3.928109	1.435697	-1.080698
H	4.957049	-2.366955	0.697902
H	2.523056	-2.874719	0.963614

20. TS1 (T1)

	X	Y	Z
C	-0.897541	-0.920130	0.340158
C	-0.194752	-1.879468	-0.387344
H	-0.425134	-0.502586	1.222179
H	-0.678231	-2.298342	-1.263361
C	-2.343403	-0.732015	0.279760
C	-2.976734	-0.062132	1.340946
C	-3.131988	-1.187074	-0.792123
C	-4.352418	0.134067	1.341551
H	-2.379099	0.307453	2.167302
C	-4.505426	-0.984924	-0.792731
H	-2.670741	-1.682041	-1.637459
C	-5.121742	-0.328076	0.274365
H	-4.823877	0.650807	2.169375
H	-5.099695	-1.335005	-1.628913
H	-6.194616	-0.173475	0.269912
C	1.136045	-2.357705	-0.127900
C	1.838350	-2.100077	1.072685
C	1.772962	-3.152131	-1.109053
C	3.118112	-2.595374	1.265508
H	1.368781	-1.529328	1.864541
C	3.056087	-3.640899	-0.913855
H	1.247275	-3.366790	-2.033123
C	3.736148	-3.362692	0.273264
H	3.639559	-2.390703	2.193379
H	3.529710	-4.238436	-1.683996
H	4.738189	-3.745042	0.429083
C	0.293970	1.712033	-0.582467
O	-0.481095	0.719142	-0.927915
C	1.410686	1.584245	0.295970
C	0.007685	3.006636	-1.129853
C	2.181828	2.669410	0.619690
C	0.776305	4.090458	-0.812098
C	1.910983	3.993549	0.090404
O	2.612237	4.986198	0.391226
H	1.656153	0.603338	0.683197
H	3.035654	2.571930	1.281260
H	0.556446	5.070554	-1.221232
H	-0.840454	3.088747	-1.799894

21. TS2 (T1)

	X	Y	Z
C	0.536599	0.544662	-1.187997
C	0.835852	-0.807241	-1.291890
H	-0.255490	0.889343	-1.843965
H	0.289249	-1.345944	-2.061863
C	1.341116	1.628165	-0.609005
C	2.740386	1.551588	-0.508440
C	0.706787	2.830178	-0.249131
C	3.476759	2.635431	-0.041852
H	3.254951	0.651378	-0.818566
C	1.443066	3.905543	0.231278
H	-0.371203	2.901960	-0.326781

C	2.831403	3.811585	0.337907
H	4.556702	2.563840	0.018754
H	0.935985	4.819242	0.519076
H	3.407024	4.653604	0.705161
C	1.699157	-1.635826	-0.481861
C	2.077202	-1.299266	0.837041
C	2.118089	-2.880934	-1.001178
C	2.867639	-2.161085	1.582578
H	1.711203	-0.382045	1.277444
C	2.925186	-3.729695	-0.257254
H	1.808795	-3.167806	-2.000697
C	3.305165	-3.371388	1.037527
H	3.136083	-1.897744	2.599160
H	3.248621	-4.674855	-0.677541
H	3.924346	-4.039129	1.625571
C	-2.153402	0.091517	0.300392
O	-0.881563	0.323843	0.475837
C	-2.714696	-0.411960	-0.911650
C	-3.041764	0.359459	1.395149
C	-4.062938	-0.623290	-1.031886
C	-4.386271	0.147160	1.278355
C	-4.986383	-0.355421	0.054802
O	-6.218688	-0.547606	-0.056150
H	-2.049408	-0.635429	-1.737420
H	-4.487682	-1.008063	-1.952467
H	-5.056251	0.350944	2.106503
H	-2.604624	0.735703	2.312830

22. TS3 (T1)

	X	Y	Z
C	-0.016353	0.404026	0.522063
C	-0.496804	-1.019548	0.477028
H	0.442993	0.574574	1.501865
H	0.292775	-1.725408	0.719547
C	-0.999997	1.534304	0.299319
C	-1.671945	2.072349	1.399894
C	-1.245131	2.059035	-0.972375
C	-2.594837	3.102842	1.232675
H	-1.477988	1.681542	2.393825
C	-2.162205	3.094656	-1.138518
H	-0.716271	1.658084	-1.827394
C	-2.843462	3.616011	-0.039040
H	-3.110462	3.509525	2.095195
H	-2.344005	3.495939	-2.129215
H	-3.555482	4.422685	-0.171319
C	-1.742638	-1.612238	0.156975
C	-2.943336	-0.925855	-0.187908
C	-1.807716	-3.039899	0.187230
C	-4.103521	-1.623901	-0.482225
H	-2.959250	0.152049	-0.222047
C	-2.971914	-3.723161	-0.108862
H	-0.911630	-3.593685	0.446551
C	-4.134561	-3.021352	-0.448002
H	-5.000558	-1.072364	-0.741518
H	-2.981302	-4.806998	-0.078751
H	-5.048719	-3.555008	-0.680254
C	2.318125	0.204092	-0.235635
O	1.044187	0.570062	-0.481216
C	2.789330	-0.370336	0.966852
C	3.221329	0.447032	-1.303809
C	4.121149	-0.686616	1.099716
C	4.545867	0.134469	-1.182601
C	5.077173	-0.453880	0.034883
O	6.288010	-0.744972	0.159499
H	2.113332	-0.570500	1.787857
H	4.500733	-1.127855	2.013914

H	5.244593	0.315915	-1.990838
H	2.822335	0.888602	-2.209653

23. TS4 (T1)

	X	Y	Z
C	-0.342600	0.469498	-0.108798
C	-1.389882	-0.259195	-0.886595
H	-0.193959	0.011840	0.865051
H	-1.534289	0.091635	-1.903624
C	-0.701559	1.931860	0.095332
C	-1.181326	2.361471	1.334977
C	-0.599665	2.853121	-0.953079
C	-1.557724	3.689763	1.527114
H	-1.261277	1.657276	2.157061
C	-0.970933	4.180354	-0.759247
H	-0.212442	2.533555	-1.913282
C	-1.453777	4.602282	0.479944
H	-1.924452	4.011009	2.495416
H	-0.881303	4.888119	-1.575723
H	-1.742071	5.636646	0.628309
C	-2.207825	-1.314421	-0.426853
C	-2.141070	-1.865367	0.885424
C	-3.169583	-1.880050	-1.315536
C	-2.969984	-2.906781	1.267455
H	-1.434206	-1.471310	1.605421
C	-3.991859	-2.919787	-0.922507
H	-3.245949	-1.479218	-2.320507
C	-3.900950	-3.444629	0.372366
H	-2.894945	-3.307994	2.272070
H	-4.710891	-3.330211	-1.622675
H	-4.545678	-4.259634	0.679147
C	2.036622	-0.146854	-0.420642
O	0.897513	0.408291	-0.883093
C	2.198823	-0.789157	0.827156
C	3.137473	-0.053191	-1.312687
C	3.420649	-1.315612	1.173998
C	4.355512	-0.574154	-0.978448
C	4.570582	-1.240013	0.294504
O	5.680510	-1.721203	0.615121
H	1.373662	-0.878746	1.520532
H	3.562359	-1.812246	2.126772
H	5.201730	-0.507235	-1.652150
H	2.973981	0.444985	-2.261299

24. TS5 (T1)

	X	Y	Z
C	-0.691727	-0.548207	-0.539345
C	-1.698330	0.557836	-0.663173
H	-0.162283	-0.661215	-1.492083
H	-2.582434	0.240209	-1.208086
C	-1.346749	-1.887764	-0.231617
C	-2.184539	-2.029854	0.879522
C	-1.100305	-2.993930	-1.046078
C	-2.762783	-3.261679	1.169624
H	-2.378745	-1.174024	1.516513
C	-1.685095	-4.228002	-0.760389
H	-0.449137	-2.894194	-1.908751
C	-2.515559	-4.363466	0.348757
H	-3.408529	-3.363831	2.034549
H	-1.488822	-5.079625	-1.401844
H	-2.969437	-5.321798	0.574451
C	-1.660420	1.921371	-0.289080
C	-0.604999	2.564177	0.422432
C	-2.779194	2.734294	-0.650170
C	-0.673597	3.912975	0.732177

H	0.255862	1.995872	0.737082
C	-2.833982	4.078315	-0.332824
H	-3.601040	2.275040	-1.189367
C	-1.779829	4.683891	0.361538
H	0.145789	4.373586	1.273082
H	-3.698363	4.664324	-0.625017
H	-1.821454	5.737661	0.610782
C	1.617209	-0.228959	0.225344
O	0.296503	-0.304709	0.502424
C	2.156372	0.148838	-1.025926
C	2.479002	-0.495212	1.318980
C	3.518467	0.230942	-1.187135
C	3.836331	-0.415103	1.170187
C	4.438200	-0.052763	-0.101337
O	5.678271	0.018334	-0.252517
H	1.504036	0.404537	-1.851398
H	3.952290	0.529628	-2.134250
H	4.508343	-0.627543	1.993360
H	2.024894	-0.773834	2.262801

25. CP1 (S0) (identical to 26. CP1 (T1))

	X	Y	Z
C	0.615657	1.036224	-0.440596
C	1.595543	0.652998	0.567950
H	1.044961	1.272641	-1.398329
H	1.271901	0.674796	1.595977
C	-0.522103	1.887056	-0.061031
C	-1.071303	2.754885	-1.023298
C	-1.138789	1.824487	1.201939
C	-2.189303	3.531013	-0.735268
H	-0.611044	2.814323	-2.005503
C	-2.260250	2.603030	1.491279
H	-0.751538	1.155929	1.963899
C	-2.790726	3.457850	0.525962
H	-2.594235	4.195137	-1.492878
H	-2.722664	2.534707	2.471392
H	-3.664411	4.063213	0.752061
C	2.886358	0.153016	0.291225
C	3.391793	-0.089384	-1.017126
C	3.756017	-0.132775	1.381193
C	4.678396	-0.565529	-1.211618
H	2.747927	0.081651	-1.870935
C	5.041613	-0.606286	1.179230
H	3.390426	0.038219	2.388811
C	5.517179	-0.825022	-0.120100
H	5.036882	-0.744075	-2.221027
H	5.681761	-0.809285	2.032329
H	6.524095	-1.197285	-0.280490
C	-1.067195	-1.156373	-0.645685
O	0.019172	-0.446603	-1.063857
C	-2.387571	-0.696343	-0.921056
C	-0.846869	-2.382500	0.051519
C	-3.467525	-1.461017	-0.539262
C	-1.914845	-3.157508	0.434878
C	-3.283042	-2.727144	0.162875
O	-4.267527	-3.424552	0.518877
H	-2.533580	0.234660	-1.460896
H	-4.485486	-1.155537	-0.758643
H	-1.782299	-4.102843	0.952087
H	0.175938	-2.691090	0.253940

27. CP2 (S0) (identical to 28. CP2 (T1))

	X	Y	Z
C	1.346802	0.626718	1.522006
C	0.509876	1.839545	1.364843

H	1.835484	0.669059	2.494440
H	0.414775	2.434930	2.262634
C	2.355620	0.201570	0.486052
C	3.022111	-1.021560	0.681338
C	2.741266	1.013921	-0.583597
C	4.023905	-1.431639	-0.194686
H	2.741159	-1.652037	1.519718
C	3.748201	0.603471	-1.462297
H	2.261513	1.977340	-0.722522
C	4.388147	-0.620280	-1.274337
H	4.526441	-2.381693	-0.032904
H	4.032247	1.247459	-2.289700
H	5.172202	-0.938550	-1.956264
C	-0.452964	2.042480	0.363459
C	-0.585536	1.233471	-0.805153
C	-1.434421	3.060735	0.562795
C	-1.649330	1.400990	-1.675968
H	0.173073	0.496071	-1.033927
C	-2.482932	3.231415	-0.323397
H	-1.356694	3.692839	1.442951
C	-2.608585	2.394120	-1.442882
H	-1.738164	0.758853	-2.547534
H	-3.219858	4.008814	-0.143071
H	-3.438718	2.521963	-2.130631
C	-0.601299	-1.093706	1.039091
O	0.332642	-0.521064	1.873809
C	-1.964405	-0.935722	1.400412
C	-0.227120	-1.932444	-0.041618
C	-2.946531	-1.613471	0.712917
C	-1.197969	-2.620055	-0.735463
C	-2.612238	-2.490083	-0.402325
O	-3.497131	-3.105970	-1.046766
H	-2.211106	-0.282574	2.232632
H	-3.994572	-1.515116	0.977843
H	-0.937971	-3.296445	-1.543757
H	0.820519	-2.061495	-0.293386

29. E-OX (S0)

	X	Y	Z
C	1.115138	-0.235486	-0.845056
C	0.035932	0.166731	0.194969
H	1.071980	0.373622	-1.754288
H	0.404742	-0.050746	1.198445
C	2.542105	-0.341817	-0.380301
C	3.061082	-1.545437	0.103148
C	3.360862	0.793356	-0.404042
C	4.375737	-1.609686	0.563526
H	2.436761	-2.430337	0.096035
C	4.669507	0.730717	0.066979
H	2.973056	1.730327	-0.791733
C	5.180954	-0.472706	0.552937
H	4.771737	-2.551338	0.927490
H	5.292581	1.617875	0.047143
H	6.202441	-0.524320	0.912415
C	-0.617093	1.520516	0.197939
C	-0.755110	2.304271	-0.954815
C	-1.127053	2.022121	1.402881
C	-1.384859	3.546257	-0.903855
H	-0.366684	1.955003	-1.904507
C	-1.763180	3.259643	1.456131
H	-1.022970	1.434336	2.309115
C	-1.893865	4.027383	0.300660
H	-1.476955	4.138436	-1.807453
H	-2.151061	3.625529	2.400081
H	-2.384241	4.993350	0.338761
C	-0.734802	-1.127311	-0.330007

O	0.463767	-1.511850	-1.075652
C	-1.881756	-0.857005	-1.251156
C	-1.057174	-2.103715	0.754327
C	-3.123126	-1.297127	-1.019870
C	-2.297859	-2.535694	1.005267
C	-3.443750	-2.131193	0.159223
O	-4.585583	-2.490067	0.407102
H	-1.662428	-0.266497	-2.134239
H	-3.947203	-1.076479	-1.689053
H	-2.520259	-3.211445	1.823603
H	-0.217118	-2.424876	1.363278

30. E-OX (T1)

	X	Y	Z
C	1.077469	-0.212517	-0.837306
C	0.047888	0.250963	0.221973
H	1.067471	0.409886	-1.739098
H	0.425674	0.033980	1.222683
C	2.502434	-0.414257	-0.392183
C	2.947972	-1.651813	0.079028
C	3.397018	0.662131	-0.425003
C	4.262161	-1.807051	0.518907
H	2.264002	-2.491526	0.077022
C	4.706227	0.509202	0.023710
H	3.067196	1.624866	-0.803381
C	5.143180	-0.727725	0.498335
H	4.598852	-2.775098	0.873701
H	5.387741	1.352270	-0.004284
H	6.164662	-0.849898	0.840638
C	-0.536848	1.635412	0.212180
C	-0.689359	2.391108	-0.957818
C	-0.975825	2.196765	1.419239
C	-1.262973	3.660866	-0.921846
H	-0.354052	1.996621	-1.910147
C	-1.554764	3.462484	1.458735
H	-0.858959	1.632784	2.339000
C	-1.700526	4.200834	0.285660
H	-1.366099	4.229048	-1.839729
H	-1.885616	3.874166	2.405747
H	-2.145478	5.189022	0.312855
C	-0.821275	-1.003790	-0.251054
O	0.347466	-1.440298	-1.071743
C	-1.995259	-0.725163	-1.118477
C	-1.130295	-1.989397	0.815631
C	-3.214740	-1.302434	-0.951018
C	-2.351883	-2.563653	0.991721
C	-3.431451	-2.228141	0.118239
O	-4.615204	-2.761127	0.297114
H	-1.853862	-0.042892	-1.948110
H	-4.039648	-1.082358	-1.616580
H	-2.530971	-3.280563	1.782949
H	-0.313908	-2.271844	1.471828

31. Z-OX (S0)

	X	Y	Z
C	0.655871	-1.244057	-1.015272
C	-0.311333	-0.009824	-1.049059
H	0.739762	-1.675185	-2.020845
H	-0.677973	0.147399	-2.063548
C	2.037512	-1.178342	-0.418571
C	2.341461	-1.832190	0.777122
C	3.048964	-0.486203	-1.094251
C	3.636010	-1.783306	1.295689
H	1.562366	-2.382133	1.290189
C	4.337577	-0.431035	-0.571959

H	2.827100	0.018068	-2.029680
C	4.635104	-1.079865	0.627290
H	3.862496	-2.299444	2.222175
H	5.110429	0.115616	-1.100631
H	5.639910	-1.040949	1.032499
C	0.032784	1.339251	-0.476800
C	0.756608	1.522625	0.710042
C	-0.414750	2.479968	-1.157469
C	1.016315	2.801549	1.196313
H	1.137074	0.668429	1.254220
C	-0.159961	3.760258	-0.671151
H	-0.973870	2.362942	-2.080336
C	0.558065	3.925192	0.510555
H	1.582731	2.919103	2.113382
H	-0.520812	4.625164	-1.216288
H	0.761426	4.919028	0.892909
C	-1.315571	-0.982989	-0.277260
O	-0.283662	-2.016421	-0.230772
C	-2.457546	-1.398929	-1.153797
C	-1.741503	-0.567790	1.093884
C	-3.741275	-1.226048	-0.822464
C	-3.022573	-0.399471	1.439024
C	-4.127988	-0.665760	0.491394
O	-5.296081	-0.462202	0.787974
H	-2.181211	-1.838098	-2.108569
H	-4.552939	-1.502927	-1.485953
H	-3.312474	-0.074765	2.432148
H	-0.948692	-0.391467	1.811145

32. Z-OX (T1)

	X	Y	Z
C	0.639924	-1.126116	-1.213918
C	-0.266243	0.146283	-1.141989
H	0.804208	-1.417466	-2.258651
H	-0.622500	0.383608	-2.145291
C	1.964404	-1.210785	-0.496264
C	2.118736	-1.991322	0.651379
C	3.075263	-0.530597	-1.009177
C	3.359724	-2.078471	1.283806
H	1.263821	-2.535199	1.033443
C	4.311263	-0.612415	-0.374937
H	2.971707	0.070988	-1.906980
C	4.457464	-1.387016	0.776779
H	3.467907	-2.692565	2.171271
H	5.161599	-0.074893	-0.779841
H	5.421281	-1.455173	1.268691
C	0.127994	1.440989	-0.486119
C	0.826225	1.522525	0.727772
C	-0.249953	2.641295	-1.105355
C	1.127141	2.757594	1.297851
H	1.157733	0.622321	1.227817
C	0.047047	3.877630	-0.536820
H	-0.787944	2.604329	-2.047356
C	0.738176	3.939823	0.671077
H	1.672840	2.794293	2.234241
H	-0.259191	4.788998	-1.038273
H	0.974769	4.899003	1.117730
C	-1.346829	-0.817916	-0.461848
O	-0.392471	-1.949917	-0.628254
C	-2.567805	-1.028909	-1.284115
C	-1.669056	-0.599550	0.972043
C	-3.836321	-0.980687	-0.795206
C	-2.935476	-0.556892	1.466621
C	-4.055882	-0.726967	0.594439
O	-5.275925	-0.646221	1.065007
H	-2.414509	-1.256861	-2.333983

H	-4.695864	-1.140140	-1.433733
H	-3.123618	-0.400704	2.521206
H	-0.839856	-0.492414	1.659577

33. Diacetyl (S0 state)

	X	Y	Z
C	-0.697608	0.344984	-0.000026
O	-0.759194	1.553672	-0.000020
C	-1.897087	-0.563248	0.000004
C	0.697605	-0.344972	-0.000005
H	-2.807594	0.033645	-0.000307
O	0.759178	-1.553660	-0.000020
C	1.897093	0.563236	0.000030
H	1.870745	1.219635	-0.874207
H	1.870547	1.219904	0.874052
H	2.807594	-0.033678	0.000199
H	-1.870439	-1.220150	-0.873832
H	-1.870748	-1.219451	0.874400

34. Diacetyl (T1 state)

	X	Y	Z
C	-0.668244	-0.315972	-0.000047
O	-0.796645	-1.551230	-0.000060
C	-1.877405	0.593315	0.000074
C	0.668304	0.316014	-0.000081
H	-2.487605	0.395711	0.885147
O	0.796652	1.551243	-0.000049
C	1.877368	-0.593353	0.000053
H	2.486913	-0.396571	0.885774
H	1.534998	-1.629668	-0.001268
H	2.488674	-0.394622	-0.883977
H	-1.535134	1.629672	-0.000189
H	-2.488045	0.395363	-0.884607

35. Diacetyl (anion doublet state)

	X	Y	Z
C	-0.655470	-0.299545	-0.000143
O	-0.864215	-1.554872	-0.000098
C	-1.856500	0.640061	0.000026
C	0.655470	0.299545	-0.000138
H	-2.480103	0.442425	0.881761
O	0.864215	1.554872	0.000168
C	1.856500	-0.640061	0.000049
H	2.479582	-0.443133	0.882319
H	1.544793	-1.685873	-0.001092
H	2.481042	-0.441451	-0.880789
H	-1.544792	1.685873	-0.000179
H	-2.480523	0.442160	-0.881347

36. (E)-form encounter complex with diacetyl (T1)

	X	Y	Z
C	1.451590	-0.240033	-0.272838
C	1.626736	-1.535045	0.057743
H	0.489123	0.076899	-0.663535
H	2.596413	-1.855926	0.429975
C	2.441761	0.834288	-0.169822
C	2.089314	2.116357	-0.628683
C	3.732509	0.661325	0.364823
C	2.986422	3.178502	-0.565767
H	1.096967	2.271072	-1.039107
C	4.627544	1.721463	0.427884
H	4.040188	-0.308942	0.736570
C	4.261343	2.986786	-0.037321

H	2.689687	4.156267	-0.928944
H	5.616872	1.563600	0.843170
H	4.962888	3.811582	0.014565
C	0.634964	-2.607813	-0.037675
C	-0.694044	-2.401333	-0.456129
C	1.019270	-3.916308	0.305646
C	-1.587818	-3.461754	-0.531166
H	-1.032199	-1.406249	-0.719752
C	0.122073	-4.977681	0.231658
H	2.038383	-4.097794	0.631935
C	-1.187584	-4.755889	-0.188346
H	-2.606106	-3.280127	-0.857385
H	0.445866	-5.976772	0.501470
H	-1.890619	-5.578949	-0.247560
C	-2.565840	1.513022	0.367502
O	-1.829525	1.114357	-0.553741
C	-2.171953	1.328169	1.816031
C	-3.850214	2.181838	0.082400
H	-1.231038	1.849322	2.011451
O	-4.590102	2.581179	0.998199
C	-4.244151	2.369004	-1.366897
H	-4.383366	3.432456	-1.577538
H	-3.455139	1.957404	-1.998544
H	-5.190704	1.858015	-1.561421
H	-2.964004	1.728252	2.451177
H	-2.017718	0.266203	2.023553

37. TS: (E)-form with diacetyl (T1)

	X	Y	Z
C	-0.060610	-0.733904	0.345677
C	1.035203	-1.055453	-0.477830
H	0.156951	-0.292793	1.310634
H	0.825143	-1.545428	-1.422028
C	-1.354877	-1.409397	0.275123
C	-2.200094	-1.368621	1.398259
C	-1.801773	-2.089652	-0.872226
C	-3.443419	-1.989279	1.381198
H	-1.873670	-0.842668	2.289291
C	-3.046393	-2.705217	-0.889128
H	-1.184515	-2.122805	-1.761215
C	-3.871958	-2.660544	0.236261
H	-4.079381	-1.947738	2.258033
H	-3.378598	-3.219822	-1.783602
H	-4.842213	-3.143502	0.218883
C	2.414727	-0.763959	-0.224173
C	2.897529	-0.247688	1.003782
C	3.364304	-1.029729	-1.241774
C	4.248142	-0.001003	1.189687
H	2.209848	-0.049059	1.815954
C	4.713993	-0.778708	-1.050544
H	3.017917	-1.429811	-2.188660
C	5.165128	-0.260782	0.165954
H	4.595574	0.393077	2.137988
H	5.419205	-0.984734	-1.847585
H	6.220161	-0.065002	0.317922
C	-0.673713	2.111648	0.012414
O	-0.636335	0.957128	-0.577935
C	0.341938	2.516747	1.039097
C	-1.733996	3.043303	-0.362906
H	1.355383	2.326061	0.674406
O	-1.797794	4.170025	0.149407
C	-2.737242	2.584672	-1.402470
H	-2.233179	2.351842	-2.345217
H	-3.242789	1.670794	-1.079584
H	-3.469028	3.375888	-1.563270
H	0.222534	3.576137	1.262557

H	0.212367	1.957732	1.975310

38. Exciplex: (E)-form with diacetyl (T1)

	X	Y	Z
C	-0.145002	-0.311277	0.195838
C	1.029654	-0.784931	-0.599264
H	0.128222	-0.215333	1.248871
H	0.808726	-1.338888	-1.505073
C	-1.318651	-1.268999	0.079729
C	-1.489803	-2.270189	1.039964
C	-2.204579	-1.201964	-0.999134
C	-2.527212	-3.193075	0.923918
H	-0.808785	-2.329540	1.883323
C	-3.245704	-2.121281	-1.112157
H	-2.085680	-0.422364	-1.742318
C	-3.408976	-3.119875	-0.153106
H	-2.650066	-3.963291	1.676995
H	-3.931607	-2.055603	-1.949307
H	-4.220710	-3.832835	-0.241869
C	2.386496	-0.551881	-0.275665
C	2.806623	0.215481	0.847114
C	3.406026	-1.102662	-1.104426
C	4.151426	0.405891	1.118359
H	2.068673	0.672686	1.494808
C	4.746212	-0.906403	-0.823541
H	3.113082	-1.688698	-1.968980
C	5.131939	-0.152193	0.290970
H	4.445227	0.998246	1.977781
H	5.500813	-1.339408	-1.470664
H	6.182132	0.001278	0.509756
C	-1.249319	1.868944	0.431936
O	-0.489389	1.022058	-0.304429
C	-1.626718	1.587997	1.845118
C	-1.616837	3.096597	-0.226131
H	-0.747841	1.529951	2.500360
O	-2.284144	3.952969	0.375049
C	-1.163897	3.314437	-1.658220
H	-0.074236	3.269012	-1.737108
H	-1.561514	2.539950	-2.320349
H	-1.516266	4.291088	-1.987600
H	-2.253966	2.407900	2.191899
H	-2.178015	0.647925	1.946701

39. Oxetane: (E)-form with diacetyl (T1)

	X	Y	Z
C	-0.683019	-0.077284	0.910498
C	0.467982	0.198096	-0.087084
H	-0.354986	-0.660835	1.777767
H	0.072705	0.252800	-1.102278
C	-1.983230	-0.637804	0.394703
C	-1.986427	-1.855611	-0.295310
C	-3.194260	0.018070	0.624902
C	-3.181877	-2.403862	-0.752968
H	-1.051543	-2.375962	-0.478723
C	-4.390848	-0.532993	0.166420
H	-3.193781	0.958556	1.162119
C	-4.388851	-1.742930	-0.524006
H	-3.171054	-3.345502	-1.290573
H	-5.325378	-0.014357	0.349961
H	-5.319387	-2.168898	-0.881701
C	1.727451	-0.623048	-0.102635
C	2.183852	-1.354868	1.001557
C	2.501564	-0.644641	-1.272362
C	3.371561	-2.081404	0.938476
H	1.612414	-1.370390	1.922367

C	3.691430	-1.364061	-1.336297
H	2.166221	-0.085675	-2.139945
C	4.131733	-2.087614	-0.229077
H	3.701580	-2.644714	1.804307
H	4.271894	-1.363140	-2.252153
H	5.055182	-2.653380	-0.277035
C	0.452677	1.646684	0.557453
O	-0.744078	1.324371	1.294687
C	1.600092	2.016511	1.482215
C	0.174848	2.812866	-0.428674
H	1.799062	1.216757	2.197183
O	1.229564	3.204591	-1.083462
C	-1.111592	2.797208	-1.235350
H	-1.061324	2.095056	-2.080816
H	-1.923092	2.504944	-0.569333
H	-1.308731	3.792958	-1.636503
H	2.505471	2.205906	0.899718
H	1.342352	2.924292	2.031062