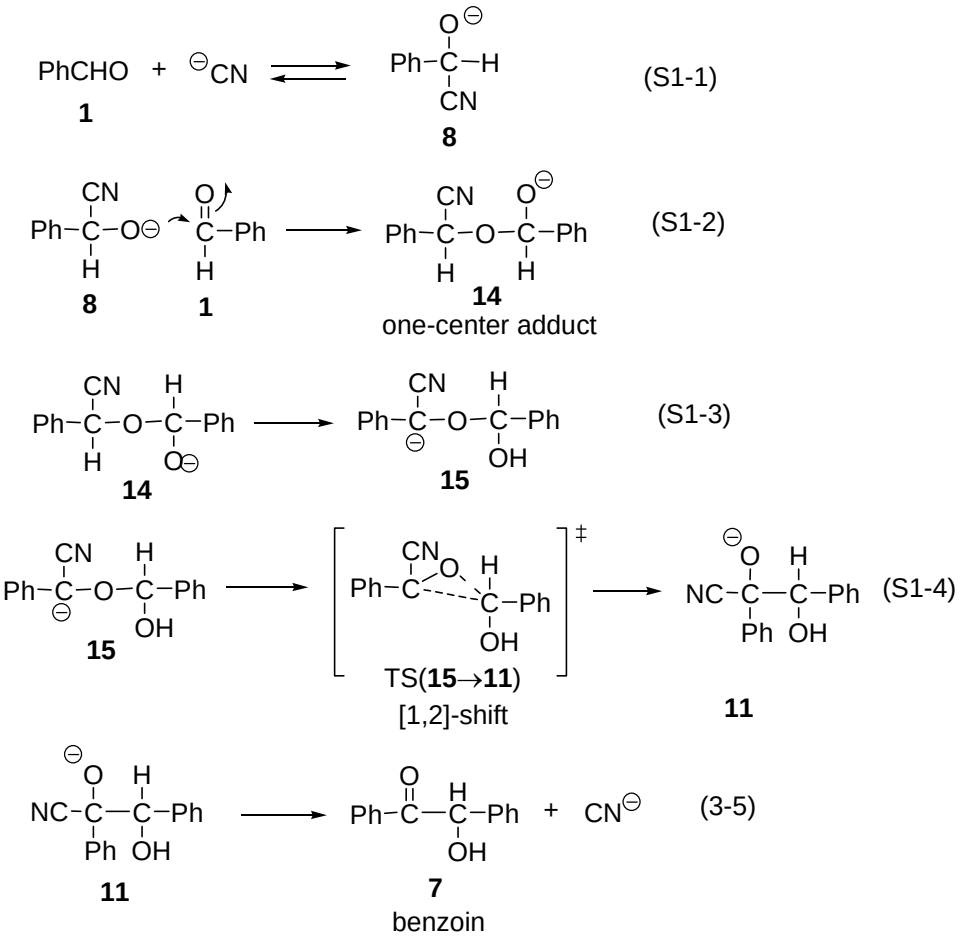
Supplementary Information

Three Competitive Transition States in the Benzoin Condensation Compared to the Clear Rate-determining Step in the Cannizzaro Reaction

Shinichi Yamabe* and Shoko Yamazaki

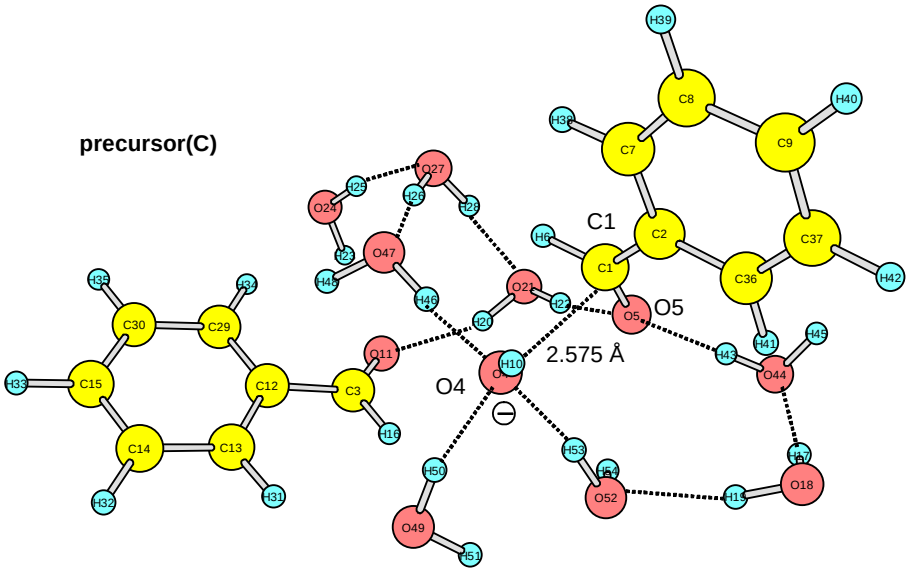
Department of Chemistry, Nara University of Education, Takabatake-cho, Nara 630-8528, Japan

yamabes@nara-edu.ac.jp

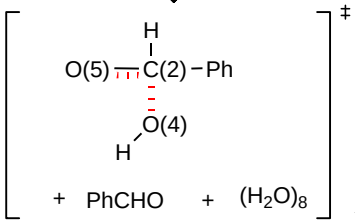


Scheme S1. An alternative route to afford the benzoin product.

precursor(C)

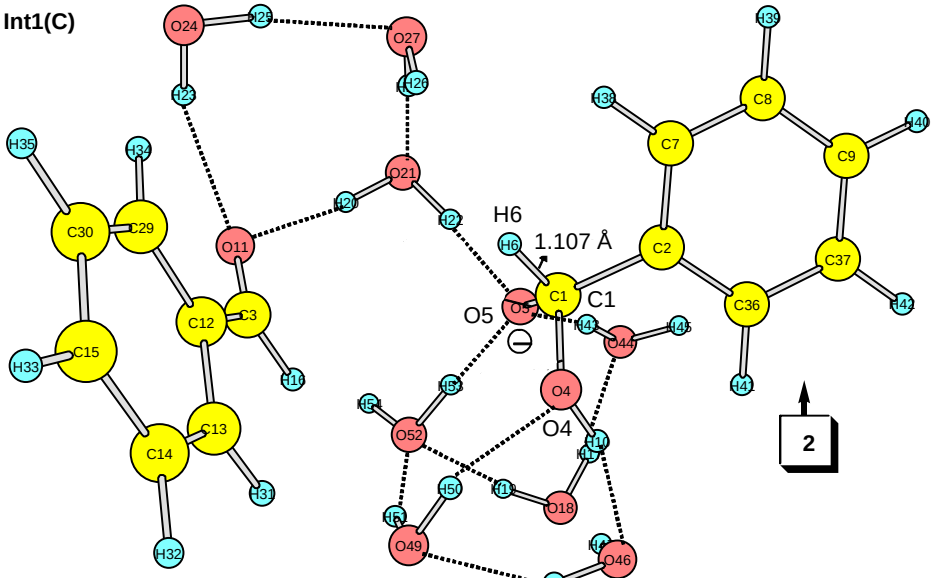


TS1(C)

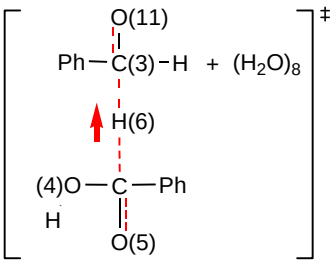


$\nu^{\ddagger}$ = 120.00i cm^{-1}

Int1(C)



TS2(C)



$\nu^{\ddagger}$ = 602.26i cm^{-1}

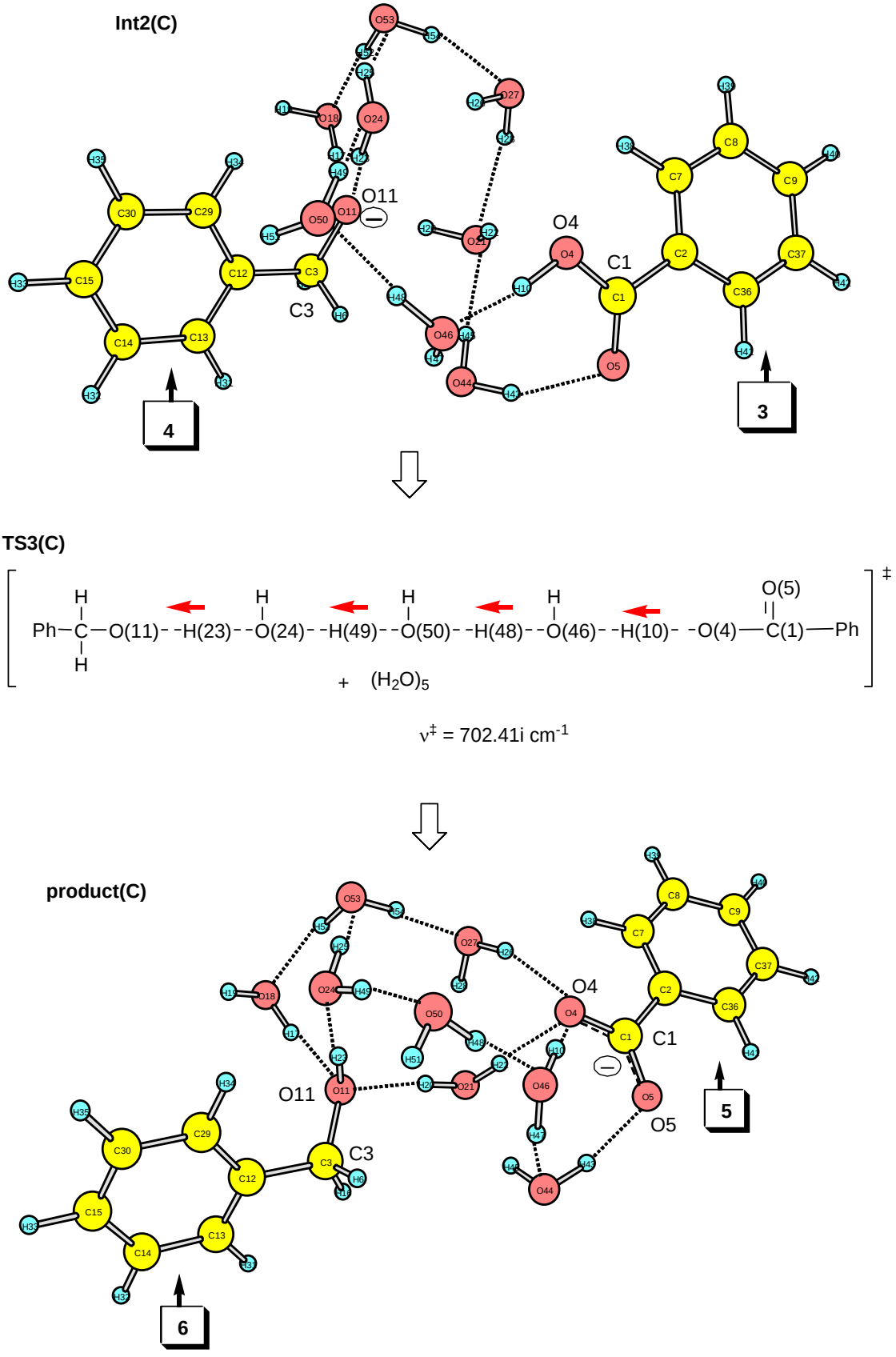
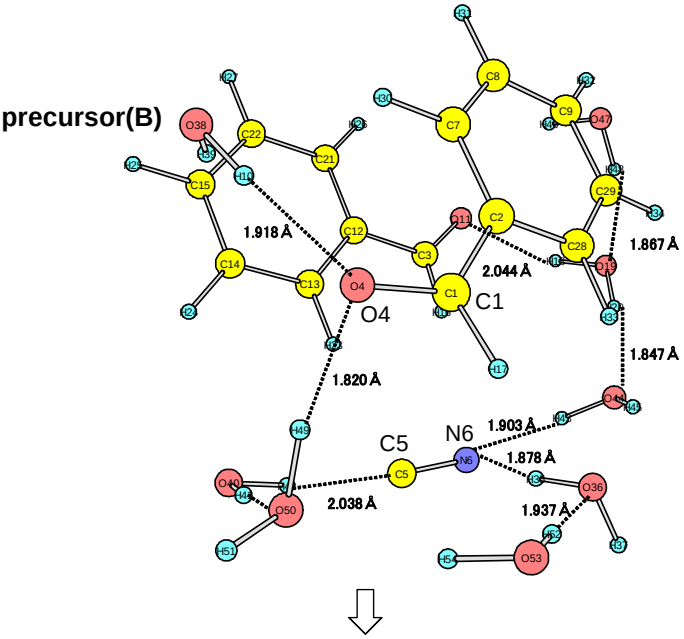
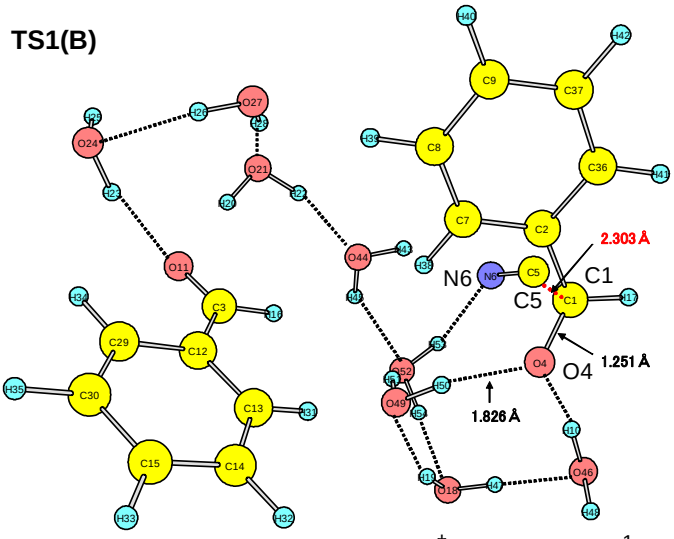


Figure S1. Geometries of the reactant-like complex (precursor) and Ints (intermediates) in Fig. 1.

precursor(B)

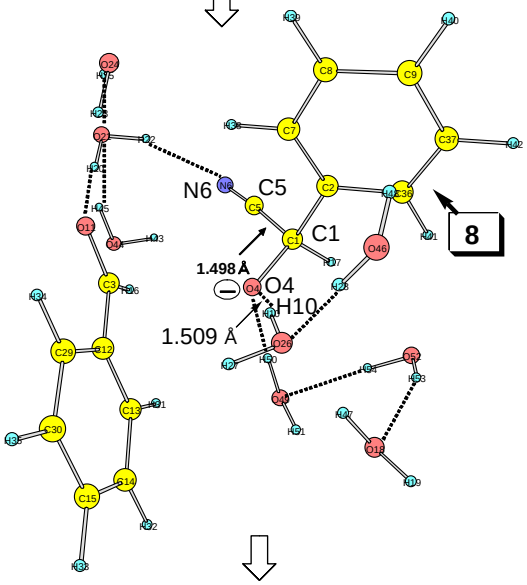


TS1(B)

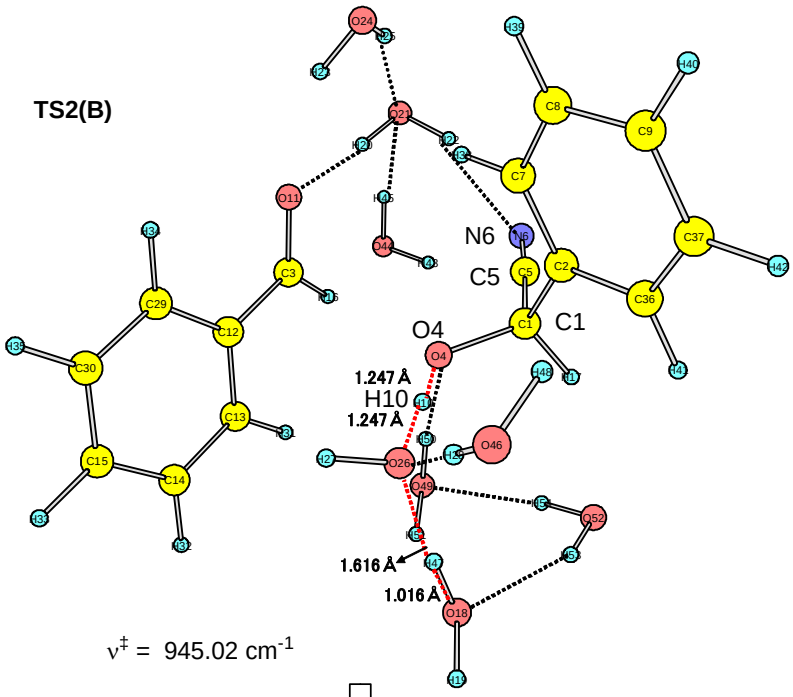


$\nu^{\ddagger}$ = 114.20i cm^{-1}

Int1(B)

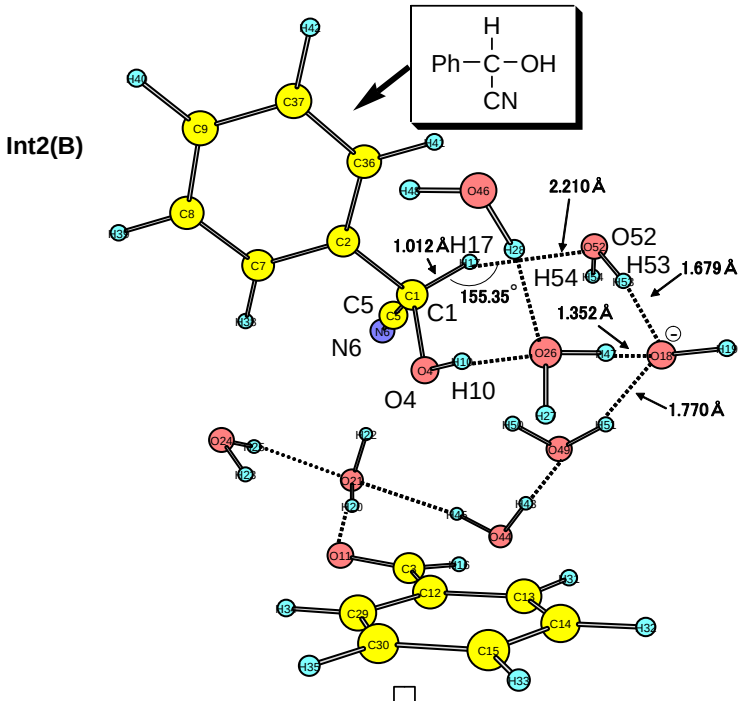


TS2(B)

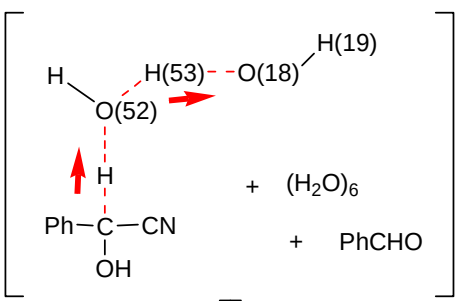


$\nu^{\ddagger}$ = 945.02 cm^{-1}

Int2(B)

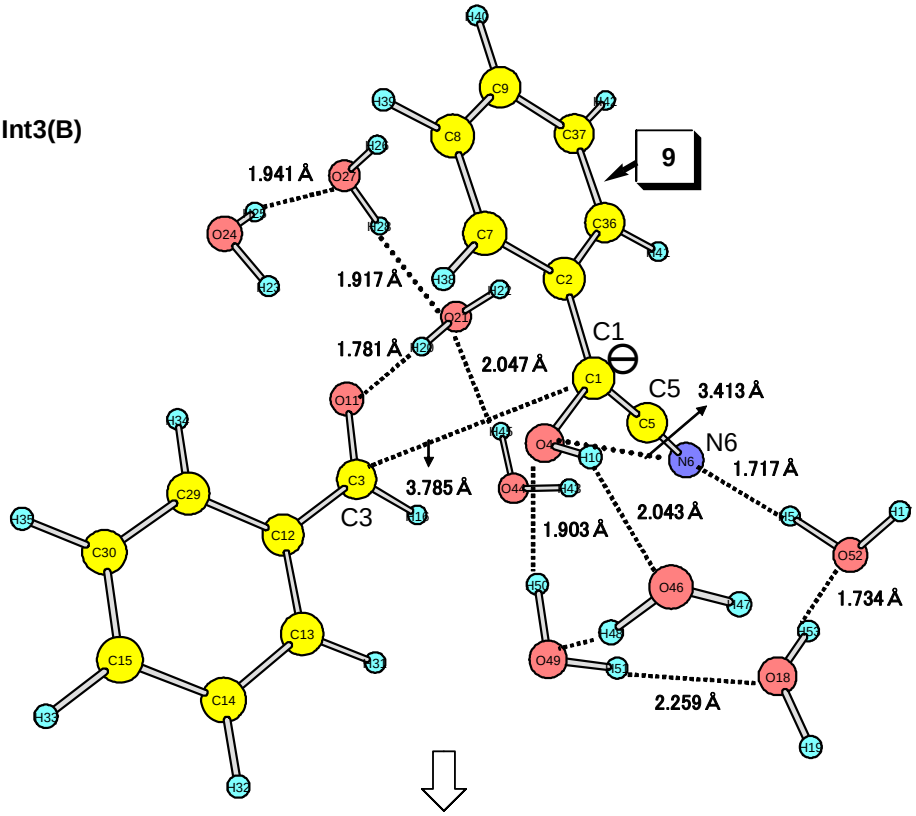


TS3(B)

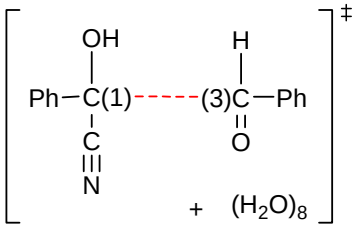


$\nu^{\ddagger}$ = 219.27i cm^{-1}

Int3(B)

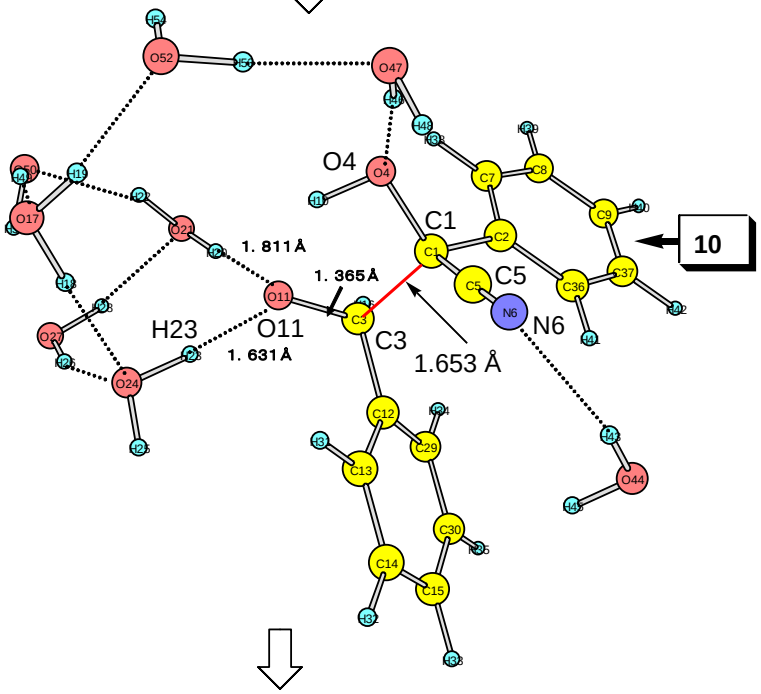


TS4(B)

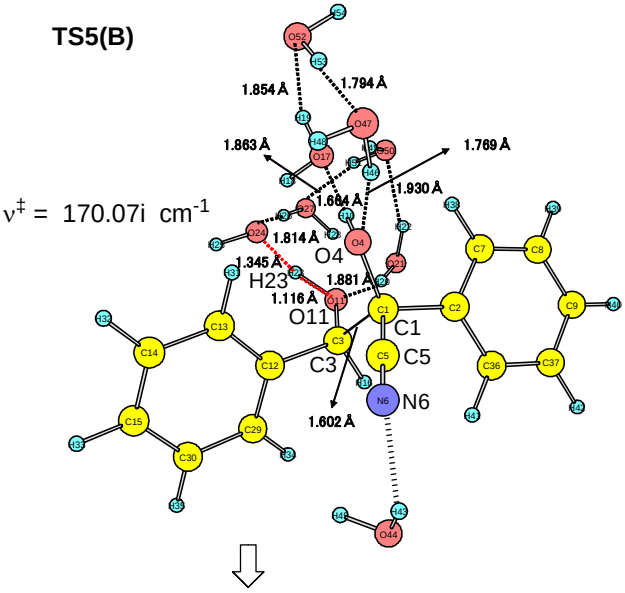


$\nu^{\ddagger}$ = 183.81i cm^{-1}

Int4(B)

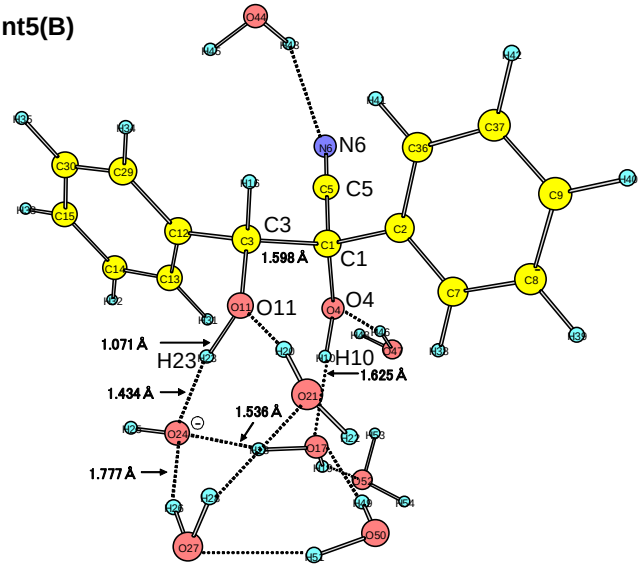


TS5(B)

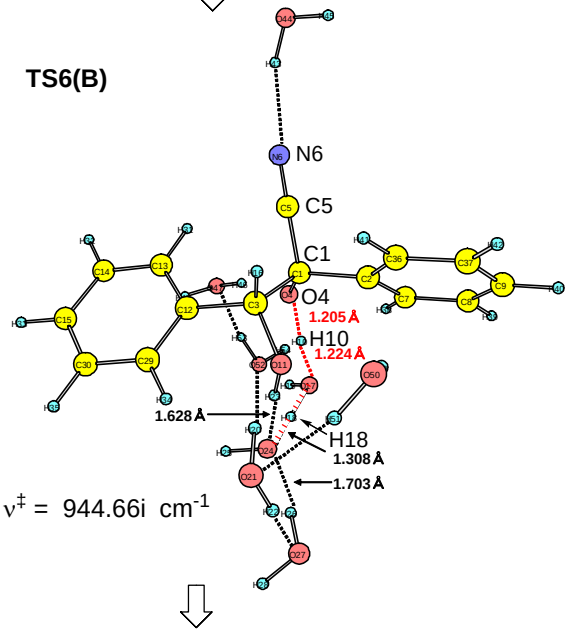


$\nu^{\ddagger}$ = 170.07i cm^{-1}

Int5(B)



TS6(B)



$\nu^{\ddagger}$ = 944.66i cm^{-1}

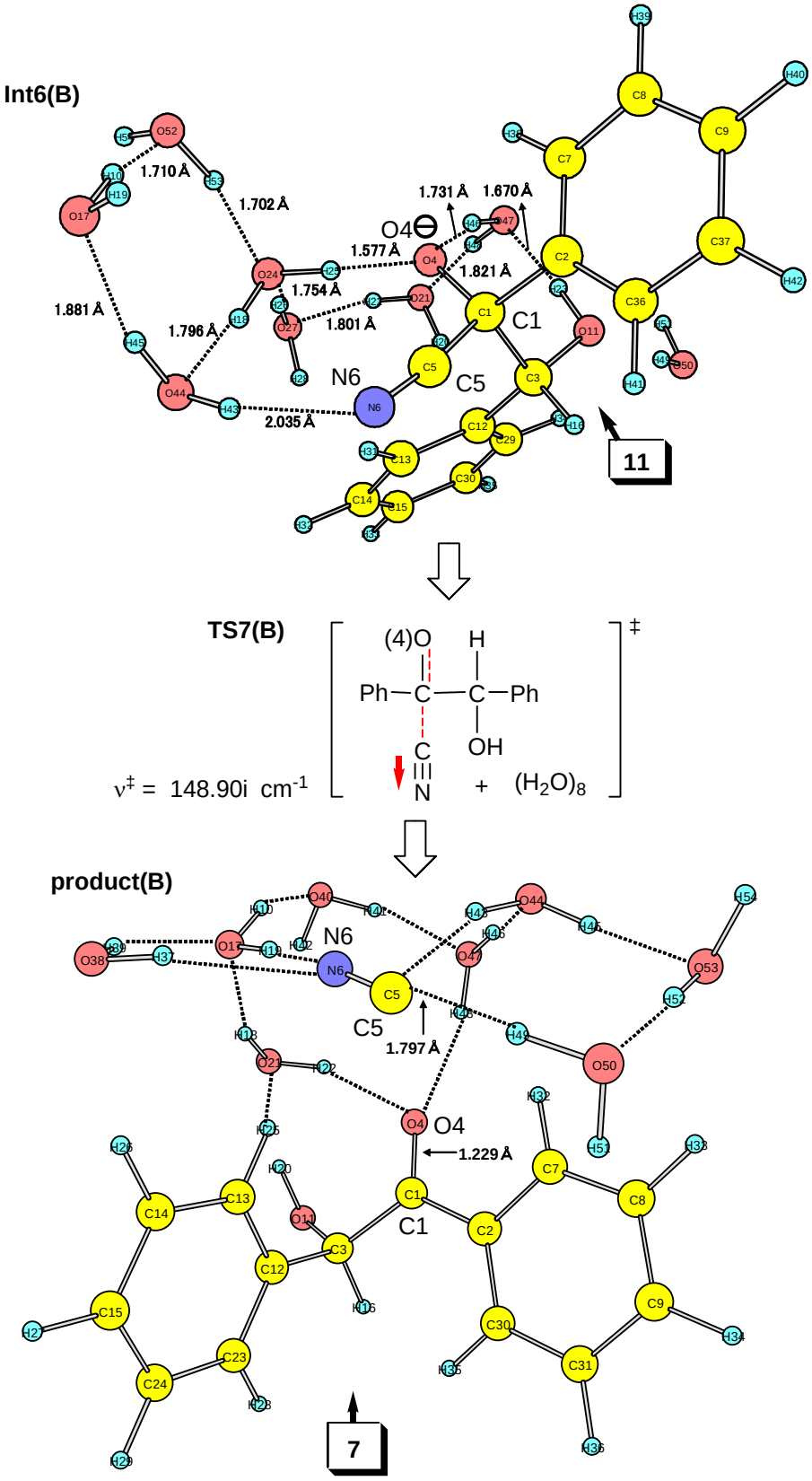
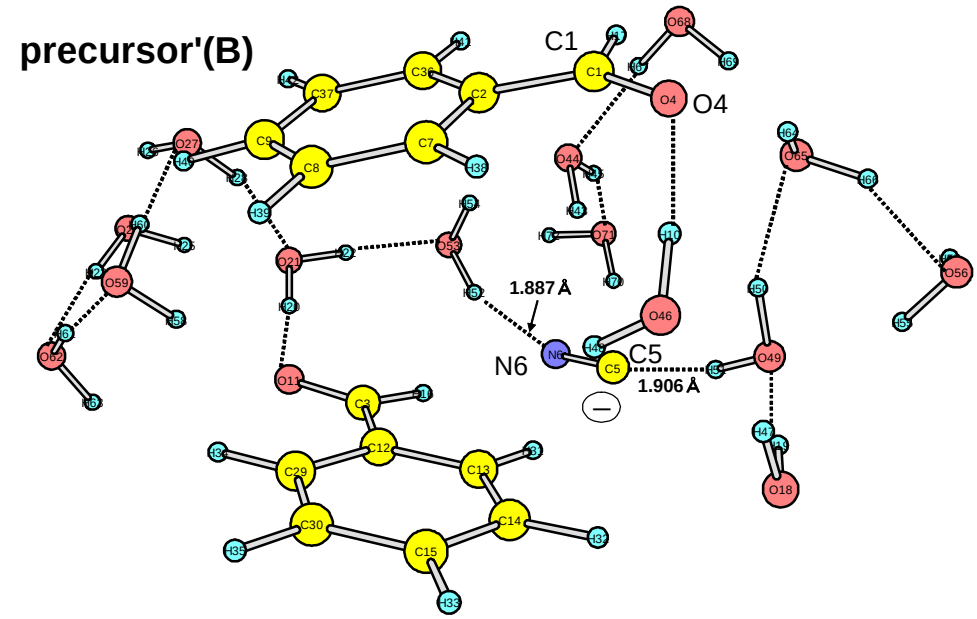
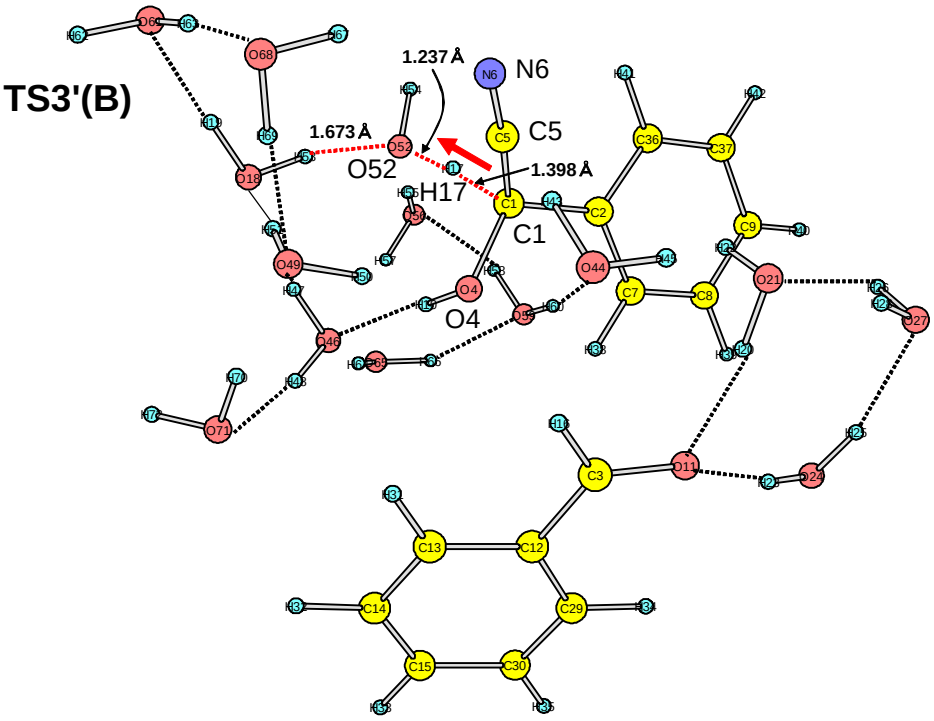


Figure S2 Geometries of the reactant-like complex (precursor) and Int1(B)-Int6(B), TS1(B), TS2(B), TS5(B), TS6(B) and product(B).


precursor'(B)
C1
O4
1.887 Å
N6
C5
1.906 Å


TS3'(B)
1.237 Å
N6
C5
1.673 Å
O52
1.398 Å
H17
C1
O4

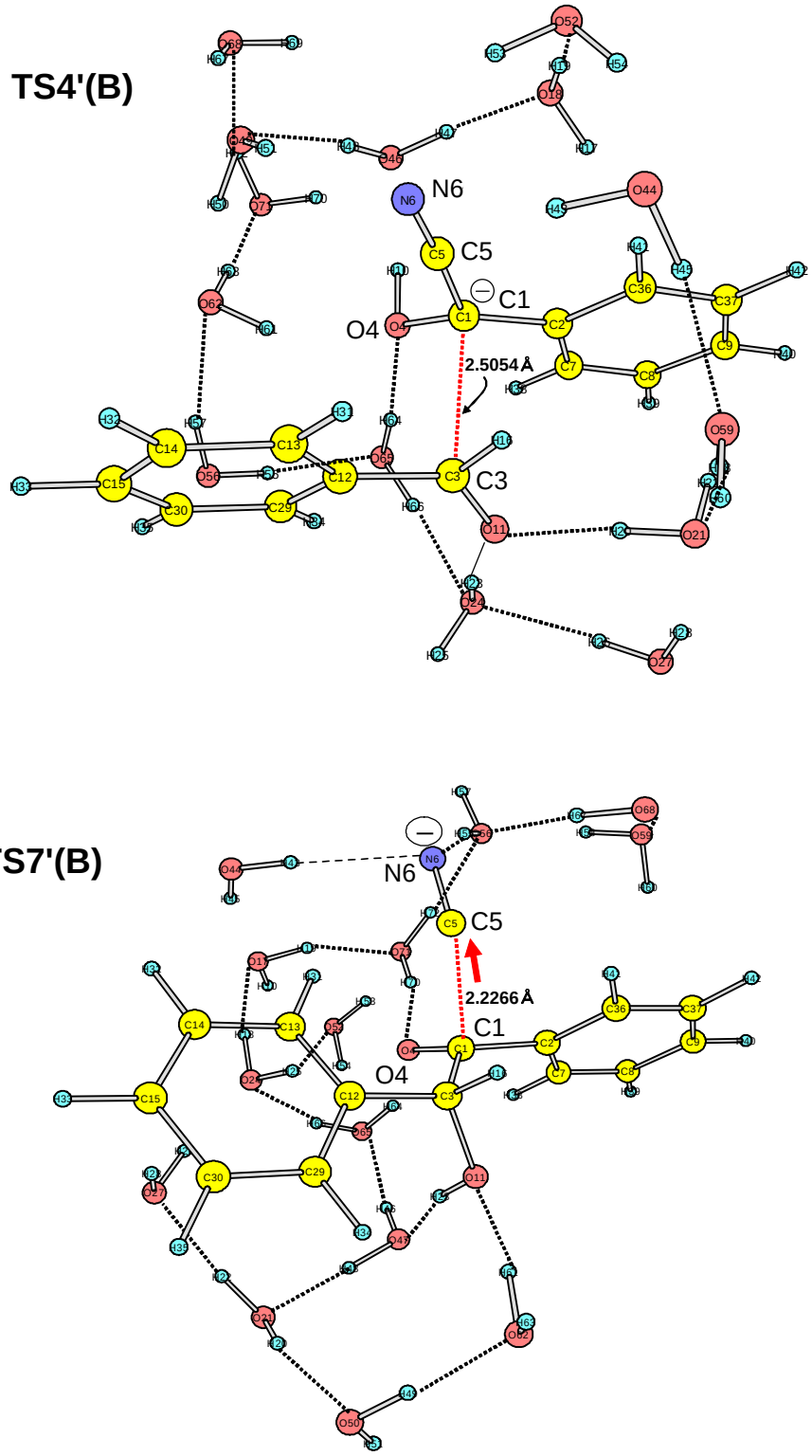
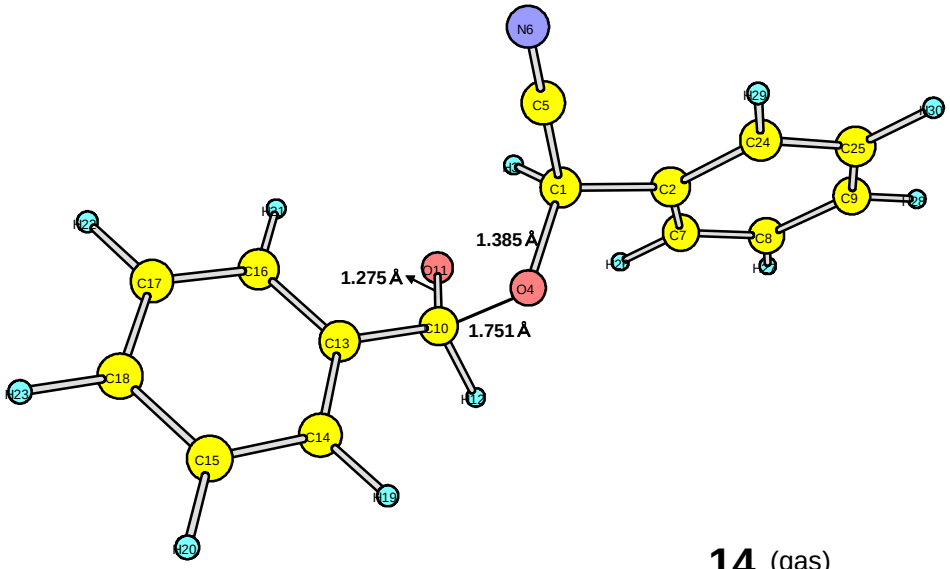
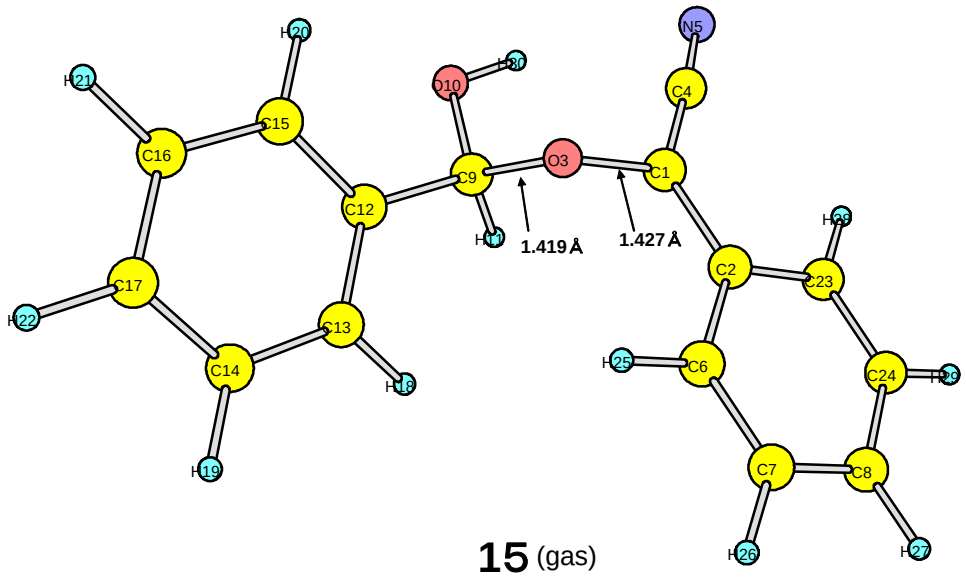


Figure S3. Geometries of extended models, precursor, TS3'(B), TS4'(B) and TS7'(B) (with large activation energies) in the benzoin condensation of (benzaldehyde)$_2$ + CN^- + $(H_2O)_{8+6}$.



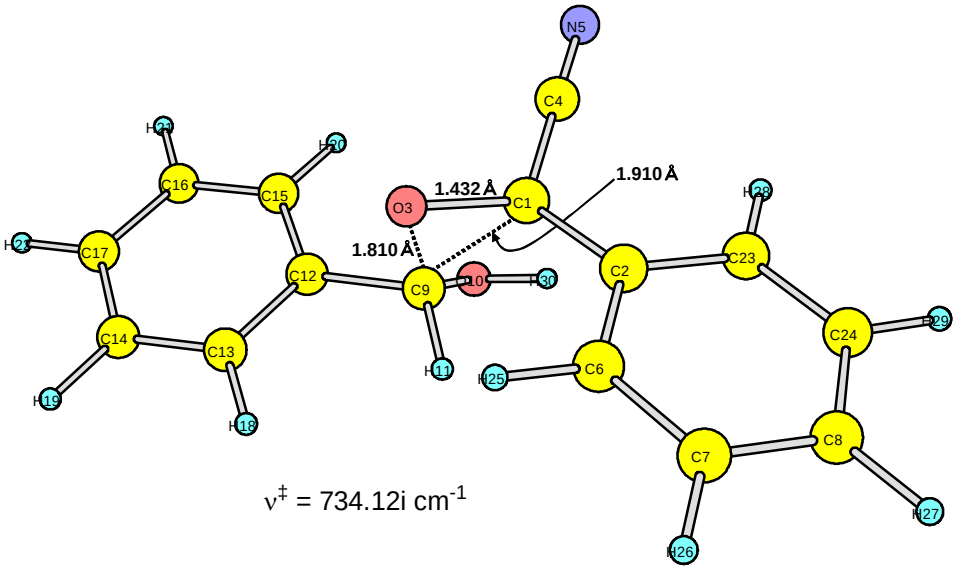
14 (gas)

ΔG' = 0 kcal/mol



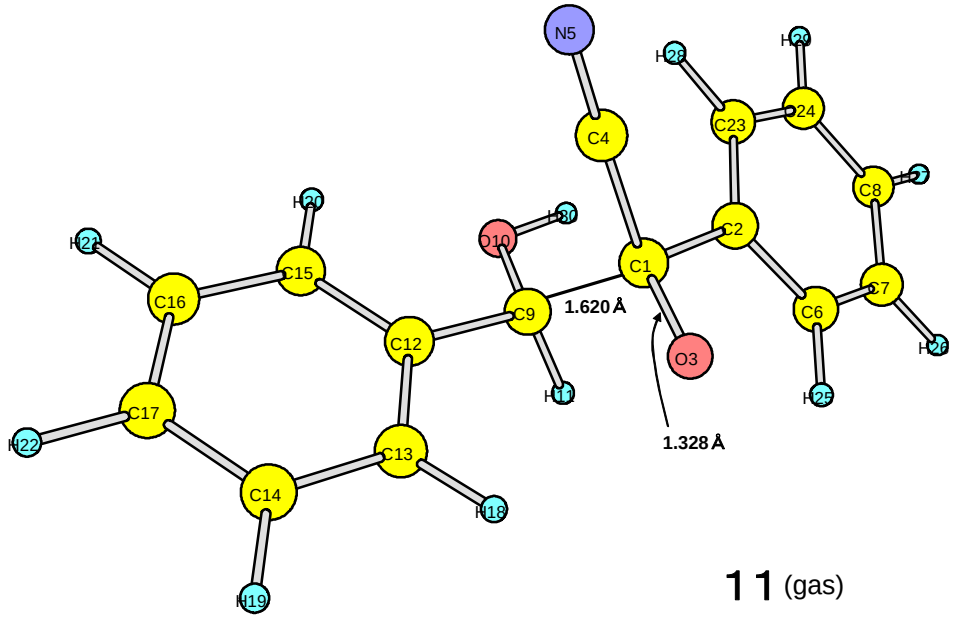
15 (gas)

ΔG' = +9.04 kcal/mol



$\nu^{\ddagger}$ = 734.12i cm^{-1}

$\Delta G'^{\ddagger}$ = +70.35 kcal/mol **TS(15→11)** (gas)



11 (gas)

$\Delta G'$ = +7.23 kcal/mol

Figure S4. Geometries of the species shown in Scheme S1, which were calculated without $(H_2O)_8$ and SCRF solvent effect, "gas". $\Delta G'$ is the Gibbs free energy relative to that of **14**.

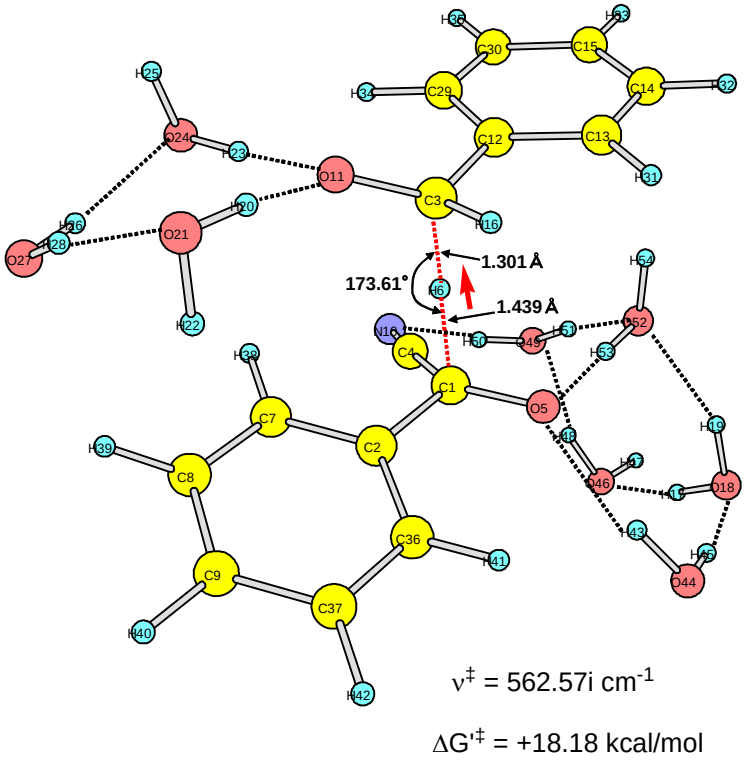
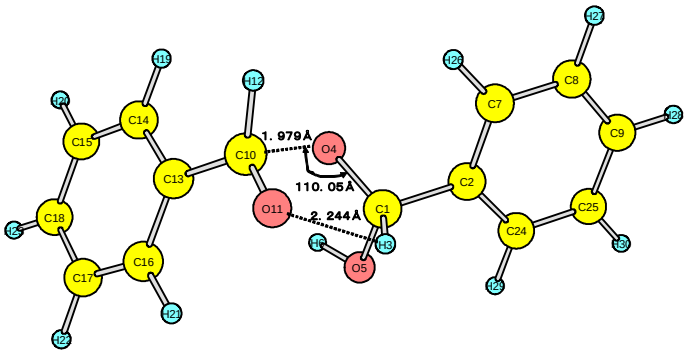


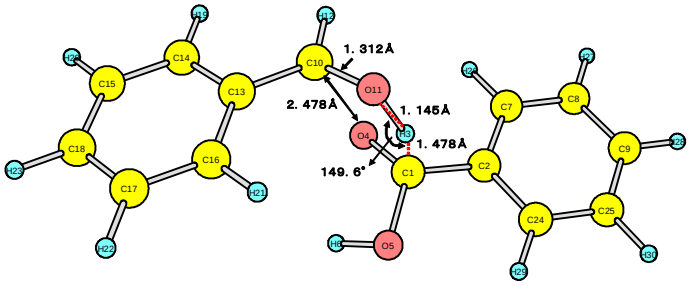
Figure S5. A hydrride-shift TS in the benzoin-condensation reacting system, **8** + **1** + $(H_2O)_8$.

Int1'(C, gas)



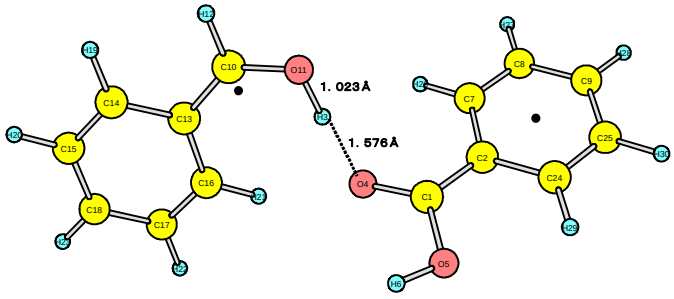
ΔG° = 0 kcal/mol

TS-SET(C, gas)



$\nu^{\ddagger}$ = 1002.04i cm^{-1} $\Delta G^{\ddagger}$ = +23.66 kcal/mol

Int-SET(C)



ΔG° = +14.77 kcal/mol

Figure S6. Geometries of the species shown in Scheme 7, which were calculated without $(H_2O)_8$ and SCRF solvent effect, "gas".

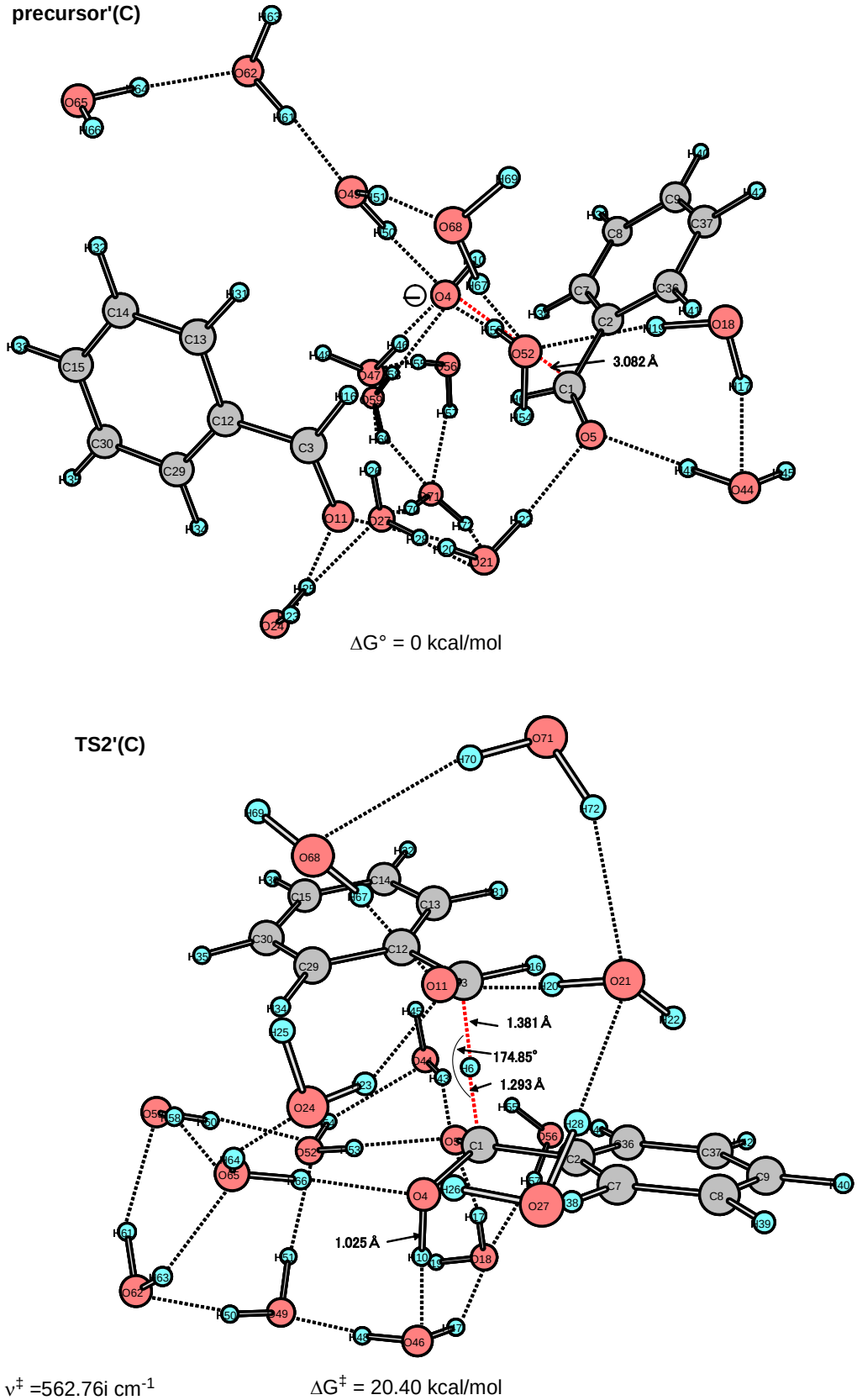


Figure S7. Geometries of expanded models, precursor and TS2'(C) in the Cannizzaro reaction.

Fig. 1
TS1(C)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.824857	-0.526435	0.186375
2	6	0	3.041780	-0.878419	-0.624344
3	6	0	-2.835686	0.826414	1.029494
4	8	0	0.950973	0.628721	-1.056053
5	8	0	1.918263	0.115490	1.279335
6	1	0	1.027815	-1.277344	0.107611
7	6	0	3.050307	-2.100889	-1.309540
8	6	0	4.168226	-2.494467	-2.047042
9	6	0	5.286145	-1.661128	-2.112737
10	1	0	1.431708	0.538317	-1.895245
11	8	0	-2.707127	0.125569	2.029805
12	6	0	-3.891343	0.658641	0.010181
13	6	0	-4.010760	1.650286	-0.980647
14	6	0	-5.012914	1.548570	-1.945138
15	6	0	-5.881378	0.454479	-1.930438
16	1	0	-2.131047	1.652951	0.831017
17	1	0	4.495127	2.371536	1.559772
18	8	0	4.552548	2.964529	0.780844
19	1	0	3.610632	3.111629	0.560741
20	1	0	-0.902017	-0.390989	2.688495
21	8	0	-0.137362	-0.987205	2.786158
22	1	0	0.612627	-0.523016	2.344136
23	1	0	-3.523532	-1.921584	2.507295
24	8	0	-3.703480	-2.763016	2.058126
25	1	0	-2.842509	-2.923278	1.598103
26	1	0	-1.212314	-2.235060	0.122204
27	8	0	-1.137264	-2.830811	0.900320
28	1	0	-0.729823	-2.262936	1.598011
29	6	0	-4.753171	-0.454627	0.012491
30	6	0	-5.743211	-0.547117	-0.961963
31	1	0	-3.300607	2.474122	-0.992165
32	1	0	-5.109205	2.313867	-2.710748
33	1	0	-6.659138	0.371732	-2.686434
34	1	0	-4.603735	-1.253083	0.739687
35	1	0	-6.405312	-1.408975	-0.974547
36	6	0	4.166637	-0.040850	-0.694165
37	6	0	5.278068	-0.435826	-1.439315
38	1	0	2.175061	-2.745077	-1.256210
39	1	0	4.164859	-3.449119	-2.567907
40	1	0	6.158571	-1.962779	-2.688301
41	1	0	4.180286	0.924160	-0.190657
42	1	0	6.141100	0.223343	-1.494673
43	1	0	3.306896	0.608193	2.224029
44	8	0	4.108628	0.897452	2.726067
45	1	0	4.773936	0.244983	2.459136
46	1	0	-0.452028	-0.389848	-1.240669
47	8	0	-1.198352	-1.040368	-1.327599
48	1	0	-2.000161	-0.503111	-1.410615
49	8	0	-0.898635	2.825820	-0.842732
50	1	0	-0.411081	2.009806	-1.093524
51	1	0	-0.209464	3.289468	-0.327055
52	8	0	1.646980	2.885684	0.408484
53	1	0	1.556048	2.097008	-0.186848
54	1	0	1.570600	2.448373	1.274059

TS2(C)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.757137	-0.321670	-0.172706
2	6	0	0.108347	-1.563559	-0.133894
3	6	0	1.096576	1.347919	-1.152305
4	8	0	-0.958262	0.277178	1.067025
5	8	0	-1.736852	-0.257503	-1.012418
6	1	0	0.190129	0.522423	-0.640840
7	6	0	1.239017	-1.614958	0.694245
8	6	0	2.086516	-2.724922	0.669264
9	6	0	1.790565	-3.807075	-0.165322
10	1	0	-1.124701	-0.402037	1.792961
11	8	0	2.276523	0.997941	-0.757172
12	6	0	0.497009	2.660261	-0.719435
13	6	0	-0.636343	3.152779	-1.381935
14	6	0	-1.210085	4.365138	-1.001369
15	6	0	-0.654021	5.100896	0.047515
16	1	0	0.822543	1.089254	-2.196834
17	1	0	-2.217090	-3.192008	0.568612
18	8	0	-3.007274	-3.065742	1.119126

19	1	0	-3.527572	-2.382312	0.630990
20	1	0	3.316353	-0.260634	-1.431182
21	8	0	3.894907	-1.032706	-1.653777
22	1	0	3.331850	-1.786064	-1.413394
23	1	0	3.124073	1.217666	0.738720
24	8	0	3.767210	1.335432	1.485122
25	1	0	4.535376	1.725171	1.039251
26	1	0	4.581884	-0.460598	1.389926
27	8	0	5.040733	-1.248341	1.034933
28	1	0	4.824959	-1.196767	0.080392
29	6	0	1.046397	3.399060	0.337035
30	6	0	0.473034	4.613042	0.713930
31	1	0	-1.070969	2.572332	-2.192311
32	1	0	-2.090466	4.735183	-1.521709
33	1	0	-1.098880	6.047291	0.346575
34	1	0	1.917446	3.015947	0.859029
35	1	0	0.905580	5.179669	1.535318
36	6	0	-0.168371	-2.644241	-0.985963
37	6	0	0.658232	-3.768818	-0.985167
38	1	0	1.472659	-0.771597	1.334467
39	1	0	3.003114	-2.704535	1.252412
40	1	0	2.447243	-4.673745	-0.183811
41	1	0	-1.025516	-2.589192	-1.650195
42	1	0	0.426937	-4.607927	-1.637206
43	1	0	-2.535437	-1.048696	-2.361882
44	8	0	-3.237890	-1.448527	-2.934377
45	1	0	-3.152285	-1.008383	-3.792314
46	8	0	-2.009951	-1.232713	2.976178
47	1	0	-2.362482	-1.996040	2.457209
48	1	0	-2.729534	-0.562156	2.910154
49	8	0	-3.679632	0.858792	2.061571
50	1	0	-2.843766	1.113852	1.624725
51	1	0	-4.142784	0.365351	1.355073
52	8	0	-4.170306	-0.873685	-0.144530
53	1	0	-3.264422	-0.531399	-0.395982
54	1	0	-4.566315	-1.054161	-1.014954

TS3(C)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.480561	-1.175912	0.211105
2	6	0	4.600994	-0.203228	-0.075794
3	6	0	-2.751746	-0.858388	-1.006905
4	8	0	2.465452	-0.675553	0.837892
5	8	0	3.588628	-2.359603	-0.167028
6	1	0	-2.313049	-1.612205	-0.334326
7	6	0	4.446519	1.165735	0.182451
8	6	0	5.491433	2.048701	-0.093921
9	6	0	6.696617	1.572814	-0.616665
10	1	0	1.629144	-1.620322	1.414639
11	8	0	-1.963472	0.323587	-0.966910
12	6	0	-4.207429	-0.632004	-0.635629
13	6	0	-5.237470	-1.083474	-1.468016
14	6	0	-6.577480	-0.891070	-1.121935
15	6	0	-6.905058	-0.232788	0.063466
16	1	0	-2.693131	-1.263434	-2.023455
17	1	0	-2.668159	1.940004	-1.374231
18	8	0	-3.137409	2.806370	-1.326132
19	1	0	-3.966628	2.563291	-0.885265
20	1	0	-0.196789	-0.095031	-1.280462
21	8	0	0.733196	-0.377529	-1.424486
22	1	0	1.188238	-0.297821	-0.558778
23	1	0	-1.677265	0.531550	0.026704
24	8	0	-1.147181	0.808007	1.351641
25	1	0	-1.503489	1.667686	1.652093
26	1	0	0.398313	1.679247	0.816193
27	8	0	0.913569	2.370014	0.331830
28	1	0	1.039040	1.966652	-0.543082
29	6	0	-4.547403	0.027468	0.556767
30	6	0	-5.884618	0.227424	0.900858
31	1	0	-4.987139	-1.585855	-2.400267
32	1	0	-7.363334	-1.247466	-1.783921
33	1	0	-7.946684	-0.076194	0.333250
34	1	0	-3.754882	0.385252	1.209931
35	1	0	-6.130249	0.741649	1.826917
36	6	0	5.805836	-0.674123	-0.611268
37	6	0	6.852571	0.208022	-0.875319
38	1	0	3.500468	1.524815	0.576910
39	1	0	5.363717	3.111267	0.099636
40	1	0	7.510870	2.263645	-0.826157
41	1	0	5.896012	-1.737056	-0.811864
42	1	0	7.788479	-0.165394	-1.285822
43	1	0	1.934888	-3.085233	-0.657703

44	8	0	0.956123	-3.135009	-0.792818
45	1	0	0.772252	-2.259867	-1.210550
46	8	0	0.891571	-2.362630	1.726439
47	1	0	0.676280	-2.791016	0.838548
48	1	0	0.035053	-1.851321	2.174876
49	1	0	-1.100856	-0.135354	2.158053
50	8	0	-0.976883	-1.127066	2.785440
51	1	0	-1.817209	-1.606565	2.726775
52	1	0	-2.150830	3.463474	0.185388
53	8	0	-1.616154	3.623798	0.993431
54	1	0	-0.702531	3.441446	0.686411

Fig. 3
TS-SET(C)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.814305	0.417250	-0.074239
2	6	0	-2.278238	0.266053	-0.200813
3	1	0	-0.411174	-1.029553	-0.340658
4	8	0	-0.091241	0.926891	-1.009621
5	8	0	-0.401358	0.598866	1.269802
6	1	0	0.576806	0.812510	1.277467
7	6	0	-2.865113	0.231050	-1.484352
8	6	0	-4.236465	0.047787	-1.634517
9	6	0	-5.061930	-0.105352	-0.515574
10	6	0	1.278651	-1.488215	-1.338736
11	8	0	0.249679	-1.877283	-0.590804
12	1	0	1.082321	-1.311699	-2.394979
13	6	0	2.600254	-1.333463	-0.826390
14	6	0	3.646112	-0.936256	-1.703052
15	6	0	4.953075	-0.803946	-1.256789
16	6	0	2.952632	-1.592914	0.528887
17	6	0	4.268963	-1.457805	0.962232
18	6	0	5.282968	-1.062550	0.080336
19	1	0	3.403705	-0.722632	-2.741458
20	1	0	5.725836	-0.487756	-1.954012
21	1	0	2.188512	-1.918149	1.227771
22	1	0	4.509521	-1.674330	2.001413
23	1	0	6.306875	-0.956316	0.428127
24	6	0	-3.119989	0.114161	0.922945
25	6	0	-4.493395	-0.067528	0.761542
26	1	0	-2.224425	0.340574	-2.353581
27	1	0	-4.665151	0.019080	-2.633469
28	1	0	-6.131794	-0.252837	-0.636793
29	1	0	-2.689455	0.157566	1.917469
30	1	0	-5.125030	-0.172141	1.640989
31	1	0	-1.025242	-3.314048	-1.143499
32	8	0	-1.718013	-3.994721	-1.118899
33	1	0	-2.095385	-3.886434	-0.221291
34	1	0	0.096723	-2.349028	1.328224
35	8	0	-0.247395	-2.136952	2.218041
36	1	0	-0.356496	-1.165307	2.155626
37	1	0	-1.902812	-2.915674	1.892096
38	8	0	-2.737614	-3.260756	1.499408
39	1	0	-3.173193	-2.460148	1.164464
40	8	0	2.160204	1.382815	1.620812
41	1	0	2.310524	1.892946	0.767763
42	1	0	2.720332	0.590223	1.536124
43	1	0	-0.854860	2.427982	-1.660781
44	8	0	-1.353099	3.275308	-1.759531
45	1	0	-2.233779	3.042513	-1.426761
46	1	0	1.480637	1.994426	-1.006308
47	8	0	2.160318	2.640109	-0.713171
48	1	0	1.634169	3.461840	-0.513502
49	1	0	0.943350	2.787387	2.528028
50	8	0	0.056215	3.192708	2.486506
51	1	0	-0.482240	2.437135	2.182693
52	1	0	0.203932	4.216788	0.896884
53	8	0	0.400551	4.602451	0.013182
54	1	0	-0.317498	4.269962	-0.572727

Fig. 4
TS1(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.423115	0.467729	-1.172553
2	6	0	-2.522746	1.639088	-1.339118
3	6	0	2.517773	-0.696586	0.883603
4	8	0	-3.020487	-0.716965	-1.207565

5	6	0	-3.823608	0.799455	1.071522
6	7	0	-3.412918	0.550973	2.145873
7	6	0	-1.162843	1.581141	-1.003327
8	6	0	-0.345042	2.695088	-1.183801
9	6	0	-0.883443	3.866890	-1.728579
10	1	0	-4.191741	-1.980532	-0.780751
11	8	0	3.271497	-0.135988	1.683794
12	6	0	2.961044	-1.346358	-0.356457
13	6	0	2.015037	-2.064459	-1.106582
14	6	0	2.412408	-2.701106	-2.282845
15	6	0	3.737816	-2.614218	-2.711866
16	1	0	1.435794	-0.727636	1.092288
17	1	0	-4.485359	0.678099	-1.349801
18	8	0	-2.802888	-3.944140	1.138881
19	1	0	-2.066014	-3.539778	0.632508
20	1	0	2.363827	1.206432	2.808615
21	8	0	1.816699	1.994690	2.976797
22	1	0	0.907812	1.624031	2.883737
23	1	0	4.677547	1.056802	1.430120
24	8	0	5.199833	1.861314	1.229901
25	1	0	5.187470	2.379266	2.048770
26	1	0	3.452434	2.677886	0.392678
27	8	0	2.545056	3.028327	0.411379
28	1	0	2.216238	2.767783	1.303166
29	6	0	4.296338	-1.261770	-0.789927
30	6	0	4.680070	-1.892746	-1.966678
31	1	0	0.984597	-2.120786	-0.754699
32	1	0	1.685531	-3.260600	-2.865213
33	1	0	4.042481	-3.106529	-3.632565
34	1	0	5.012823	-0.694575	-0.203902
35	1	0	5.708606	-1.823455	-2.310713
36	6	0	-3.054512	2.820177	-1.870673
37	6	0	-2.234523	3.929041	-2.076771
38	1	0	-0.763919	0.674954	-0.559005
39	1	0	0.697366	2.668234	-0.871570
40	1	0	-0.245336	4.736727	-1.864959
41	1	0	-4.114885	2.866658	-2.112115
42	1	0	-2.651570	4.842973	-2.493952
43	1	0	-1.372244	0.836594	2.251560
44	8	0	-0.470017	0.503287	2.444350
45	1	0	-0.667305	-0.360111	2.854146
46	8	0	-4.705492	-2.815061	-0.645830
47	1	0	-3.592120	-3.607944	0.656457
48	1	0	-4.484449	-3.330549	-1.436565
49	8	0	-0.957815	-2.011373	0.161965
50	1	0	-1.579550	-1.478162	-0.381859
51	1	0	-1.164113	-1.736563	1.087185
52	8	0	-2.005184	-1.842883	2.789062
53	1	0	-2.686268	-1.139163	2.679620
54	1	0	-2.410756	-2.664725	2.418154

TS2(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.370393	-0.162330	1.212339
2	6	0	-2.446397	-0.082630	0.127798
3	6	0	1.965922	1.600670	-0.090771
4	8	0	-0.080600	-0.403635	0.716342
5	6	0	-1.319566	1.131066	1.947130
6	7	0	-1.226430	2.155638	2.489701
7	6	0	-2.427654	0.939326	-0.829658
8	6	0	-3.388136	0.978924	-1.838251
9	6	0	-4.378449	-0.005794	-1.902807
10	1	0	-0.045266	-1.405771	-0.025266
11	8	0	1.403766	2.498662	-0.717621
12	6	0	2.760058	0.541698	-0.741948
13	6	0	3.324949	-0.478935	0.036608
14	6	0	4.088786	-1.473461	-0.575807
15	6	0	4.294709	-1.446662	-1.957080
16	1	0	1.934556	1.595255	1.008753
17	1	0	-1.665416	-0.931745	1.947878
18	8	0	0.601730	-4.065810	1.321110
19	1	0	0.620602	-4.987840	1.027188
20	1	0	0.464353	3.706926	0.284732
21	8	0	-0.137714	4.355981	0.715785
22	1	0	-0.739583	3.789780	1.235959
23	1	0	-0.230039	3.256328	-2.050497
24	8	0	-1.032001	3.802666	-2.020703
25	1	0	-0.946863	4.230656	-1.146155
26	8	0	0.111615	-2.449736	-0.689181
27	1	0	0.892221	-2.275680	-1.237650
28	1	0	-1.187517	-3.016790	-1.780320
29	6	0	2.965598	0.562320	-2.130654

30	6	0	3.731386	-0.428217	-2.735872
31	1	0	3.124963	-0.524200	1.104628
32	1	0	4.513545	-2.273377	0.024299
33	1	0	4.889051	-2.223845	-2.431713
34	1	0	2.514030	1.360463	-2.711624
35	1	0	3.888560	-0.415268	-3.811285
36	6	0	-3.442278	-1.062242	0.065105
37	6	0	-4.404753	-1.026572	-0.949181
38	1	0	-1.670433	1.716857	-0.801103
39	1	0	-3.351953	1.786380	-2.564223
40	1	0	-5.128022	0.022524	-2.690351
41	1	0	-3.454786	-1.858837	0.805127
42	1	0	-5.173573	-1.794681	-0.990286
43	1	0	0.915269	2.845494	3.148743
44	8	0	1.646337	3.386691	2.807984
45	1	0	1.175879	4.013135	2.225490
46	8	0	-1.926648	-3.290381	-2.381762
47	1	0	0.422719	-3.510087	0.490255
48	1	0	-2.603845	-2.612969	-2.230792
49	8	0	1.510991	-1.587205	2.648738
50	1	0	0.976307	-1.097845	1.972096
51	1	0	1.564617	-2.485405	2.270765
52	8	0	-1.071884	-2.735861	3.305585
53	1	0	-0.805536	-3.377936	2.620390
54	1	0	-0.236242	-2.234949	3.405126

TS3(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.496343	0.721114	0.580952
2	6	0	2.291615	-0.365710	-0.047030
3	6	0	-2.278200	-1.447290	0.637010
4	8	0	0.100193	0.736659	0.213272
5	6	0	1.608010	0.795922	2.002658
6	7	0	1.722009	0.916446	3.163868
7	6	0	1.733163	-1.237081	-1.002739
8	6	0	2.500843	-2.238264	-1.608137
9	6	0	3.851336	-2.384342	-1.291748
10	1	0	-0.005375	1.207671	-0.643645
11	8	0	-1.884539	-2.500643	0.133096
12	6	0	-3.408904	-0.673600	0.092095
13	6	0	-3.736516	0.561934	0.667118
14	6	0	-4.795063	1.310753	0.153583
15	6	0	-5.535668	0.819114	-0.922534
16	1	0	-1.788172	-1.060208	1.545781
17	1	0	2.162454	2.089121	0.185944
18	8	0	0.474683	4.585920	-0.560988
19	1	0	0.747314	5.458373	-0.879531
20	1	0	-0.324701	-3.066342	0.924232
21	8	0	0.571022	-3.351101	1.214553
22	1	0	1.160491	-2.741319	0.732967
23	1	0	-0.879774	-3.878950	-1.347065
24	8	0	-0.122591	-4.475190	-1.461905
25	1	0	0.306718	-4.418575	-0.588168
26	8	0	2.604935	3.085722	-0.078046
27	1	0	3.075676	3.351399	0.729197
28	1	0	4.052107	2.615248	-1.203402
29	6	0	-4.152747	-1.159705	-0.995778
30	6	0	-5.215484	-0.417753	-1.497095
31	1	0	-3.147153	0.948808	1.492769
32	1	0	-5.028800	2.279037	0.586022
33	1	0	-6.360770	1.402936	-1.323669
34	1	0	-3.875885	-2.116095	-1.428652
35	1	0	-5.792404	-0.791583	-2.339109
36	6	0	3.659569	-0.533669	0.267412
37	6	0	4.423049	-1.522308	-0.347826
38	1	0	0.682123	-1.140296	-1.254358
39	1	0	2.014307	-2.924249	-2.296141
40	1	0	4.448347	-3.161847	-1.761266
41	1	0	4.115429	0.113875	1.012860
42	1	0	5.472494	-1.627474	-0.079952
43	1	0	0.247584	-0.775879	3.393898
44	8	0	-0.375559	-1.518502	3.297471
45	1	0	0.128802	-2.188073	2.794762
46	8	0	-0.947778	2.444284	-1.799497
47	1	0	-0.375411	3.235136	-1.737981
48	1	0	-1.550555	2.584972	-1.037524
49	8	0	-1.573728	2.972647	0.902380
50	1	0	-0.981756	2.194527	0.982804
51	1	0	-0.956533	3.709706	0.734022
52	8	0	4.869542	2.215824	-1.565970
53	1	0	1.324640	4.078191	-0.366195
54	1	0	4.697223	1.267124	-1.458252

Fig. 5
TS4(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.126249	0.482564	-0.217816
2	6	0	1.257122	0.957773	-0.021642
3	6	0	-0.118284	-1.344538	0.903189
4	8	0	-0.461317	0.025071	-1.503013
5	6	0	-1.144066	1.235195	0.418622
6	7	0	-1.996159	1.782687	1.019273
7	6	0	2.290696	0.382790	-0.784552
8	6	0	3.623870	0.722472	-0.554866
9	6	0	3.957020	1.660308	0.427576
10	1	0	-0.354310	0.780983	-2.149250
11	8	0	0.993203	-1.909120	0.632881
12	6	0	-1.411570	-1.936806	0.443932
13	6	0	-2.589945	-1.702358	1.169657
14	6	0	-3.794873	-2.279851	0.765676
15	6	0	-3.838036	-3.096193	-0.365940
16	1	0	-0.199124	-0.815880	1.869706
17	1	0	0.755336	3.606517	-0.824595
18	8	0	0.161530	4.181970	-1.334348
19	1	0	-0.552011	4.419331	-0.692882
20	1	0	2.518129	-1.737761	1.536815
21	8	0	3.418566	-1.600923	1.921231
22	1	0	3.617690	-0.688072	1.656272
23	1	0	1.624733	-2.979404	-0.594891
24	8	0	2.131375	-3.597988	-1.182058
25	1	0	2.250526	-4.396491	-0.647023
26	1	0	3.924046	-2.732996	-1.003895
27	8	0	4.743080	-2.447894	-0.555310
28	1	0	4.419357	-2.258374	0.350046
29	6	0	-1.461195	-2.762655	-0.690601
30	6	0	-2.666956	-3.334014	-1.091844
31	1	0	-2.571421	-1.069489	2.053796
32	1	0	-4.698898	-2.092837	1.340432
33	1	0	-4.777397	-3.544701	-0.681410
34	1	0	-0.552638	-2.943251	-1.254348
35	1	0	-2.693829	-3.966427	-1.976149
36	6	0	1.606524	1.900576	0.969002
37	6	0	2.939314	2.250691	1.184600
38	1	0	2.038455	-0.355206	-1.536658
39	1	0	4.400728	0.201548	-1.105995
40	1	0	4.996357	1.925567	0.603790
41	1	0	0.828706	2.348585	1.583733
42	1	0	3.182803	2.982573	1.951644
43	1	0	-2.622344	1.171566	2.860459
44	8	0	-2.651388	0.765566	3.749260
45	1	0	-1.743551	0.446084	3.863165
46	8	0	-0.780972	2.167173	-3.100390
47	1	0	-0.494310	2.952828	-2.581112
48	1	0	-1.727014	2.030587	-2.876203
49	8	0	-3.162209	0.957054	-2.099514
50	1	0	-2.511866	0.242078	-1.947938
51	1	0	-3.323638	1.280125	-1.198076
52	8	0	-1.822811	4.623711	0.571737
53	1	0	-2.059850	3.682069	0.735655
54	1	0	-1.394231	4.898935	1.396234

TS5(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.404555	0.867169	0.607578
2	6	0	-0.517825	2.050685	0.273035
3	6	0	0.887553	0.186220	-0.759216
4	8	0	-0.193233	-0.075363	1.476980
5	6	0	1.579253	1.384018	1.349829
6	7	0	2.506156	1.807236	1.908059
7	6	0	-1.898330	1.950869	0.458907
8	6	0	-2.731088	3.016141	0.110308
9	6	0	-2.192624	4.187888	-0.419925
10	1	0	-0.874250	-0.672383	1.029980
11	8	0	-0.200817	-0.433625	-1.351961
12	6	0	2.111338	-0.714355	-0.605409
13	6	0	2.181697	-1.765728	0.321472
14	6	0	3.320283	-2.568850	0.398379
15	6	0	4.408041	-2.342455	-0.448179

16	1	0	1.197635	1.033469	-1.387485
17	8	0	-2.011340	-1.877981	0.879959
18	1	0	-1.519709	-2.445499	0.189304
19	1	0	-2.085039	-2.369324	1.729244
20	1	0	-1.682018	0.055564	-2.403946
21	8	0	-2.555944	0.072007	-2.846652
22	1	0	-3.176304	-0.130600	-2.109866
23	1	0	-0.298632	-1.540607	-1.254036
24	8	0	-0.712868	-2.813520	-1.127137
25	1	0	0.025275	-3.438117	-1.150818
26	1	0	-2.068742	-2.938584	-2.325785
27	8	0	-2.859592	-2.753289	-2.889842
28	1	0	-2.687699	-1.828731	-3.179209
29	6	0	3.207032	-0.503252	-1.455003
30	6	0	4.347474	-1.306481	-1.380360
31	1	0	1.342417	-1.947740	0.982575
32	1	0	3.357175	-3.376675	1.125513
33	1	0	5.292880	-2.971160	-0.383525
34	1	0	3.152504	0.288158	-2.200581
35	1	0	5.182438	-1.124738	-2.052977
36	6	0	0.021884	3.225610	-0.269538
37	6	0	-0.812805	4.288655	-0.610686
38	1	0	-2.326621	1.039505	0.860123
39	1	0	-3.804960	2.918806	0.245005
40	1	0	-2.844021	5.014875	-0.692070
41	1	0	1.095149	3.310087	-0.429694
42	1	0	-0.382210	5.195296	-1.028604
43	1	0	3.624113	2.863168	0.373946
44	8	0	3.867464	2.884653	-0.567368
45	1	0	3.971086	1.940913	-0.767260
46	1	0	-0.562986	-0.146348	3.205570
47	8	0	-0.714864	-0.452250	4.131668
48	1	0	0.152767	-0.798409	4.391283
49	1	0	-3.526310	-1.419850	-0.182247
50	8	0	-4.166440	-1.269390	-0.907304
51	1	0	-3.900131	-1.960296	-1.563110
52	8	0	-2.337663	-2.629871	3.547091
53	1	0	-1.773044	-1.870318	3.837728
54	1	0	-3.240092	-2.278881	3.593907

TS6(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.720123	0.817243	0.121725
2	6	0	-2.084590	0.119904	0.377105
3	6	0	0.108608	-0.015694	-0.956874
4	8	0	-0.012925	1.066527	1.289224
5	6	0	-1.088727	2.143002	-0.471563
6	7	0	-1.396289	3.169627	-0.918370
7	6	0	-2.523976	-0.073185	1.688723
8	6	0	-3.760572	-0.673597	1.939146
9	6	0	-4.573526	-1.083292	0.883711
10	1	0	0.258578	0.146650	2.019852
11	8	0	0.053928	-1.387696	-0.648435
12	6	0	1.549930	0.463157	-1.192764
13	6	0	1.941031	1.809591	-1.123497
14	6	0	3.256611	2.194181	-1.396284
15	6	0	4.212836	1.242661	-1.753911
16	1	0	-0.427770	0.084255	-1.909963
17	8	0	0.633829	-0.679414	2.841773
18	1	0	1.129195	-1.482306	2.210916
19	1	0	1.308800	-0.223253	3.400815
20	1	0	0.542617	-2.842004	-1.736877
21	8	0	0.706691	-3.744603	-2.075626
22	1	0	0.814340	-4.259491	-1.241087
23	1	0	0.651333	-1.644704	0.130528
24	8	0	1.576172	-2.305032	1.296732
25	1	0	2.486344	-2.052347	1.078962
26	1	0	1.283269	-3.932375	0.887614
27	8	0	1.191979	-4.843341	0.484807
28	1	0	2.106708	-5.160836	0.449008
29	6	0	2.518469	-0.480305	-1.573496
30	6	0	3.832378	-0.095605	-1.848216
31	1	0	1.224621	2.578249	-0.860927
32	1	0	3.526421	3.246017	-1.333646
33	1	0	5.236499	1.542498	-1.965232
34	1	0	2.240185	-1.523749	-1.674283
35	1	0	4.557814	-0.850893	-2.141215
36	6	0	-2.910595	-0.283794	-0.681374
37	6	0	-4.142271	-0.886965	-0.430448
38	1	0	-1.890581	0.236158	2.510833
39	1	0	-4.081676	-0.825086	2.966936

40	1	0	-5.532300	-1.557388	1.079775
41	1	0	-2.593922	-0.150908	-1.711387
42	1	0	-4.756044	-1.212803	-1.265882
43	1	0	-2.155230	4.915004	-1.675096
44	8	0	-2.775193	5.592457	-2.004366
45	1	0	-3.631958	5.161269	-1.872440
46	1	0	1.219666	2.186710	1.708292
47	8	0	2.037896	2.639077	2.047915
48	1	0	2.703023	2.377685	1.391061
49	1	0	-2.045877	-2.643454	-1.580193
50	8	0	-2.047457	-3.035069	-2.467746
51	1	0	-1.176515	-3.487033	-2.484135
52	8	0	2.283058	1.057827	4.263006
53	1	0	2.297107	1.686580	3.491947
54	1	0	1.602654	1.430496	4.844262

TS7(B)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.931750	-0.524892	-0.112955
2	6	0	-2.392834	-0.933040	-0.186671
3	6	0	0.097395	-1.479031	-0.778686
4	8	0	-0.549042	0.136890	0.882081
5	6	0	-1.152002	0.974204	-1.746199
6	7	0	-1.257823	2.079045	-2.134354
7	6	0	-3.269850	-0.396801	0.763620
8	6	0	-4.621101	-0.740933	0.764137
9	6	0	-5.116324	-1.636358	-0.184364
10	1	0	-1.286200	4.656574	0.047425
11	8	0	-0.001217	-2.703454	-0.041642
12	6	0	1.543898	-0.979115	-0.849923
13	6	0	1.871099	0.339850	-1.193746
14	6	0	3.201343	0.748348	-1.322095
15	6	0	4.239972	-0.158247	-1.097003
16	1	0	-0.234542	-1.714100	-1.793112
17	8	0	-0.618084	4.357634	-0.606744
18	1	0	0.032204	3.193731	0.697338
19	1	0	-1.048066	3.672493	-1.177102
20	1	0	3.203716	-1.159135	1.735566
21	8	0	2.909294	-0.893999	2.623055
22	1	0	2.766568	0.081950	2.525277
23	1	0	0.205177	-2.513509	0.920020
24	8	0	0.009190	2.707410	1.556857
25	1	0	-0.300448	1.798864	1.321534
26	1	0	1.715384	2.145415	1.956255
27	8	0	2.633052	1.786415	1.955956
28	1	0	2.794345	1.617894	1.011860
29	6	0	2.595406	-1.887884	-0.646303
30	6	0	3.928811	-1.478337	-0.763620
31	1	0	1.090709	1.063105	-1.381919
32	1	0	3.394477	1.776693	-1.617159
33	1	0	5.277020	0.154878	-1.193036
34	1	0	2.378326	-2.925924	-0.415157
35	1	0	4.723842	-2.203896	-0.605368
36	6	0	-2.898471	-1.833722	-1.134271
37	6	0	-4.247415	-2.182537	-1.132132
38	1	0	-2.874493	0.295617	1.499131
39	1	0	-5.286671	-0.308773	1.507721
40	1	0	-6.169283	-1.908578	-0.185903
41	1	0	-2.242016	-2.268132	-1.880080
42	1	0	-4.620683	-2.885126	-1.873397
43	1	0	0.700369	2.979893	-2.672179
44	8	0	1.474509	3.531085	-2.455034
45	1	0	1.098636	4.136719	-1.793339
46	1	0	-0.115019	-1.195443	2.374221
47	8	0	0.401346	-2.004168	2.549152
48	1	0	1.324536	-1.648936	2.652714
49	1	0	0.775864	-4.382797	-0.271121
50	8	0	1.310617	-5.185789	-0.099042
51	1	0	1.394395	-5.173985	0.866440
52	8	0	-1.864428	4.747665	1.900095
53	1	0	-1.355693	3.913058	2.024835
54	1	0	-1.268667	5.421571	2.262411