Supplementary Information

A New Mechanism of a Favorskii Rearrangement

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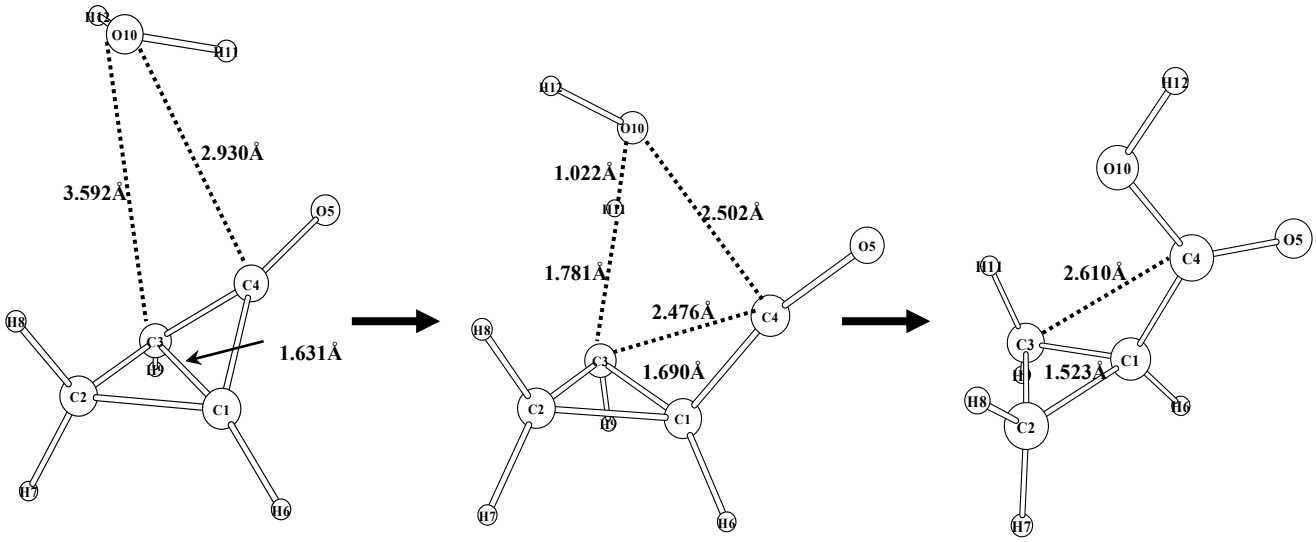
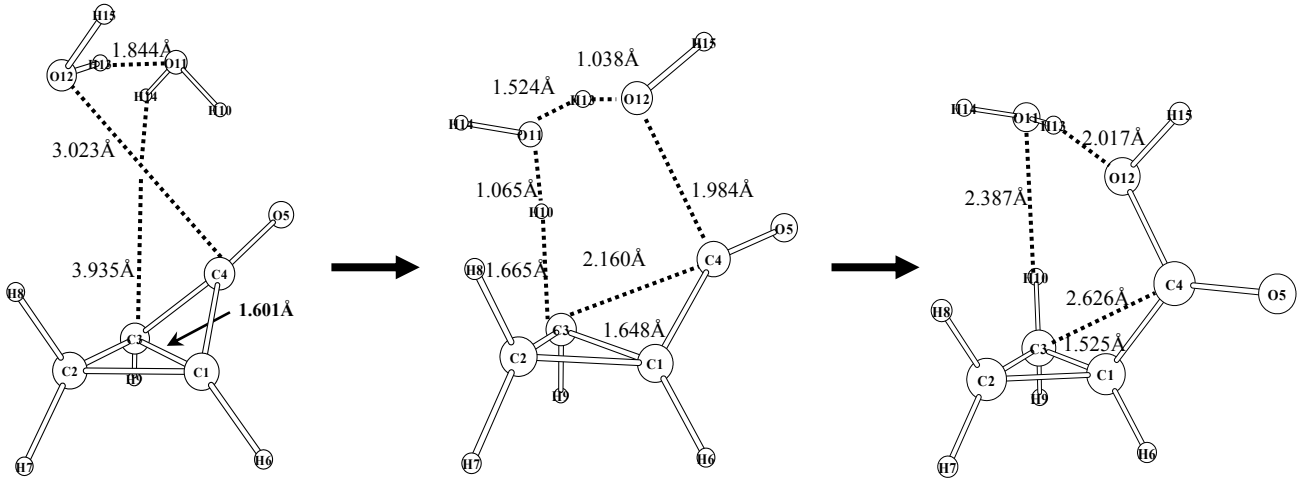


before TS
ΔE= 0 kcal/mol

ts3B
ΔE‡= 37.47 kcal/mol

after TS
ΔE= -45.35 kcal/mol

Figure S1-1



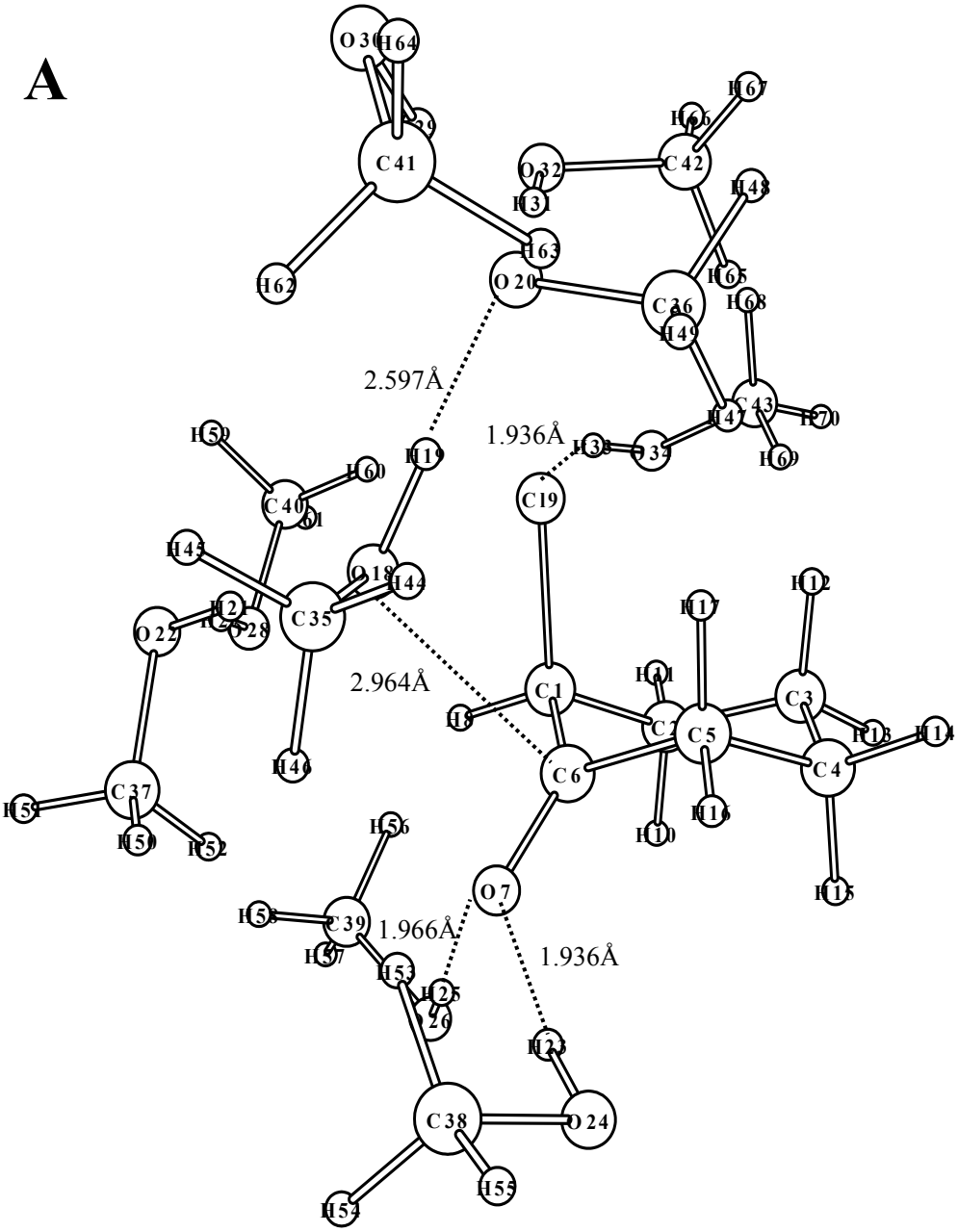
before TS
ΔE= 0 kcal/mol

ts3B+H_2O
ΔE‡= 31.77 kcal/mol

after TS
ΔE= -39.76 kcal/mol

Figure S1-2

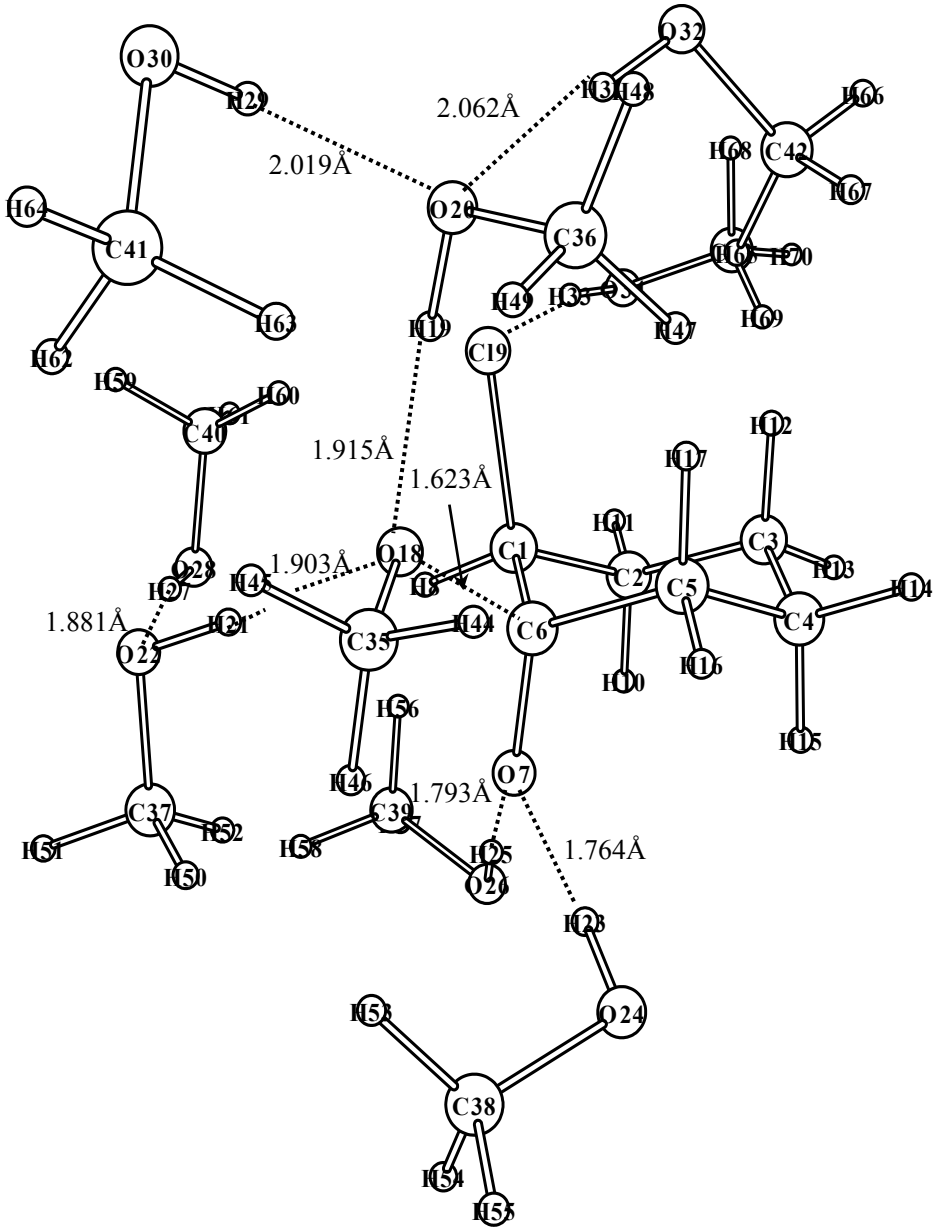
Figure S1. Optimized geometries of ts3B and ts3B+H_2O. ts3B was reported in Ref. 9c, and ts3B+H_2O was obtained in this work. $\Delta E^{\ddagger}$ is the energy difference between ts3B (or ts3B+H_2O) and the preceding intermediate, I2B (or I2B+H_2O). See Scheme 6 in the text.



precursor

ΔE= 0 kcal/mol

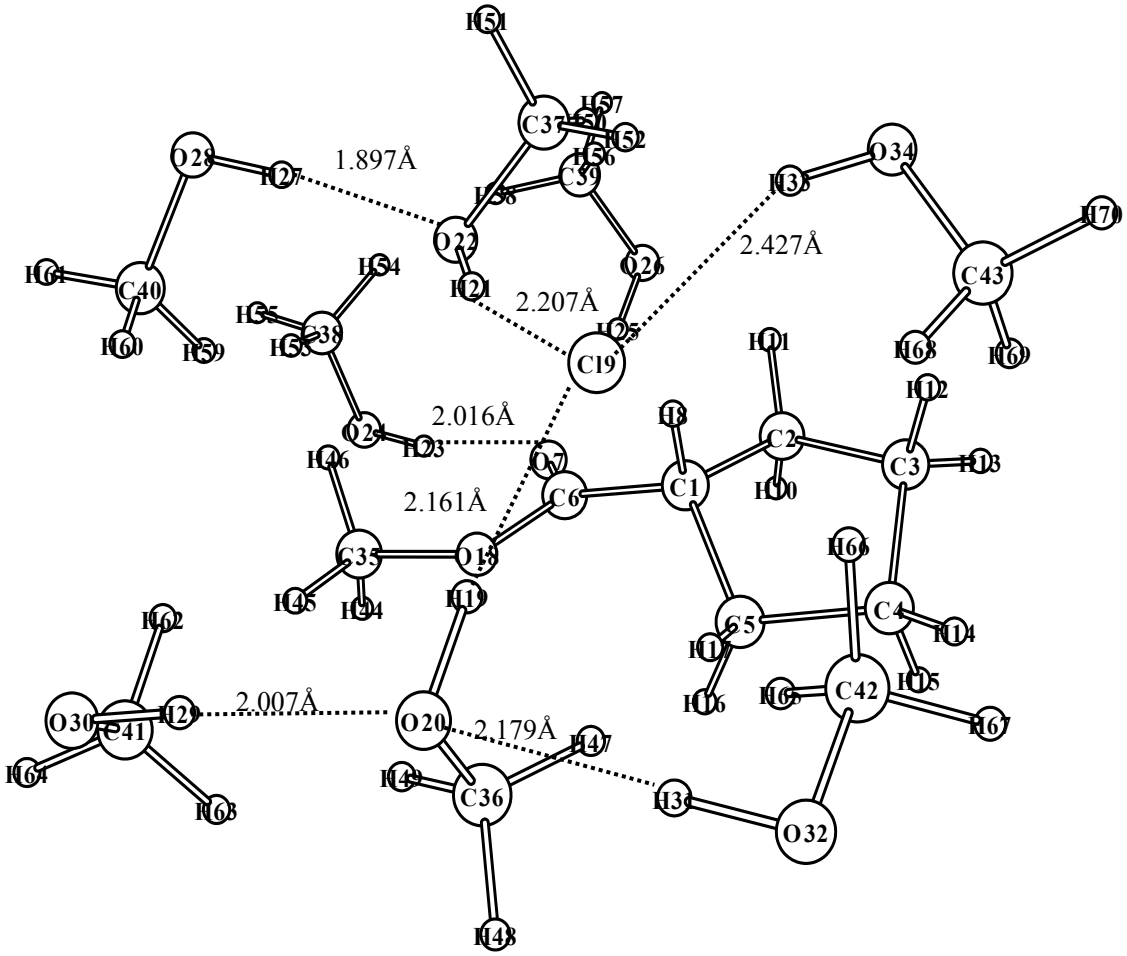
Figure S2-1



IntA

ΔE= -1.07 kcal/mol

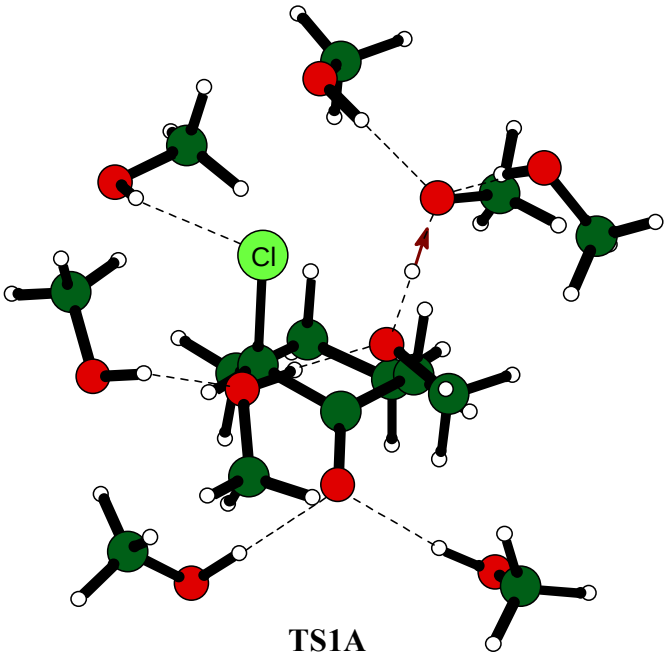
Figure S2-2



product

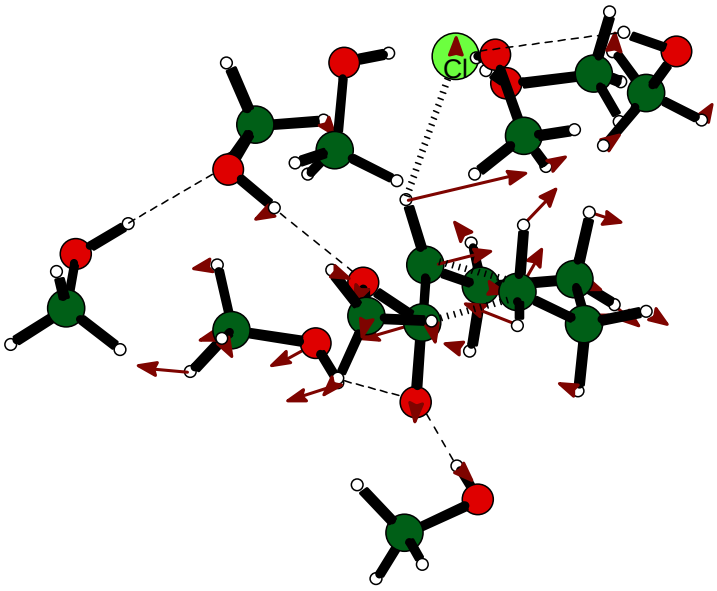
ΔE= -27.83 kcal/mol

Figure S2-3



TS1A
$\Delta E^{\ddagger}$ = +2.77 kcal/mol
$\nu^{\ddagger}$ = 950.87*i* cm^{-1}

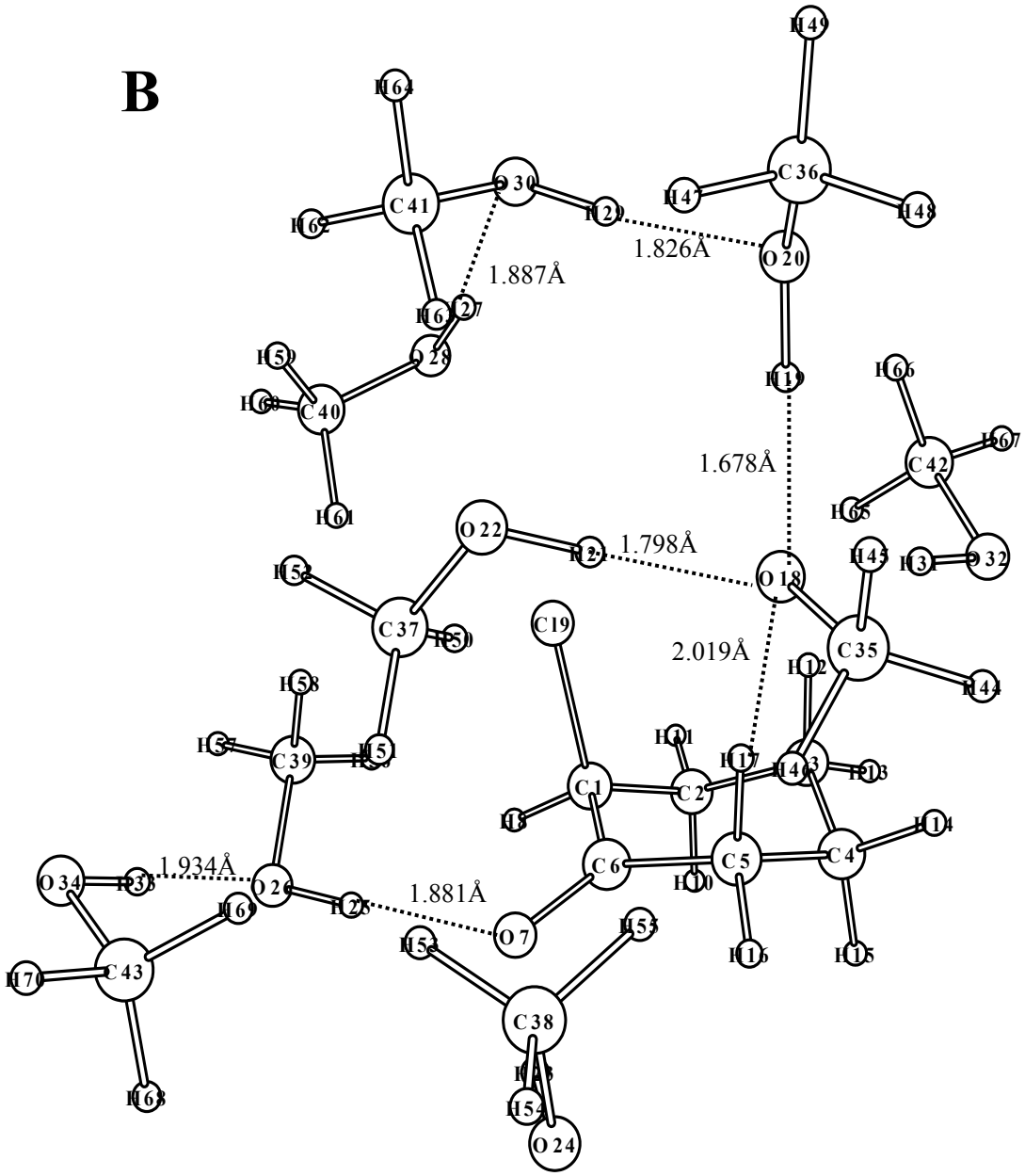
Figure S2-4



TS2A
$\Delta E^{\ddagger}$ =+33.79 kcal/mol
$\nu^{\ddagger}$ = 361.27*i* cm^{-1}

Figure S2-5

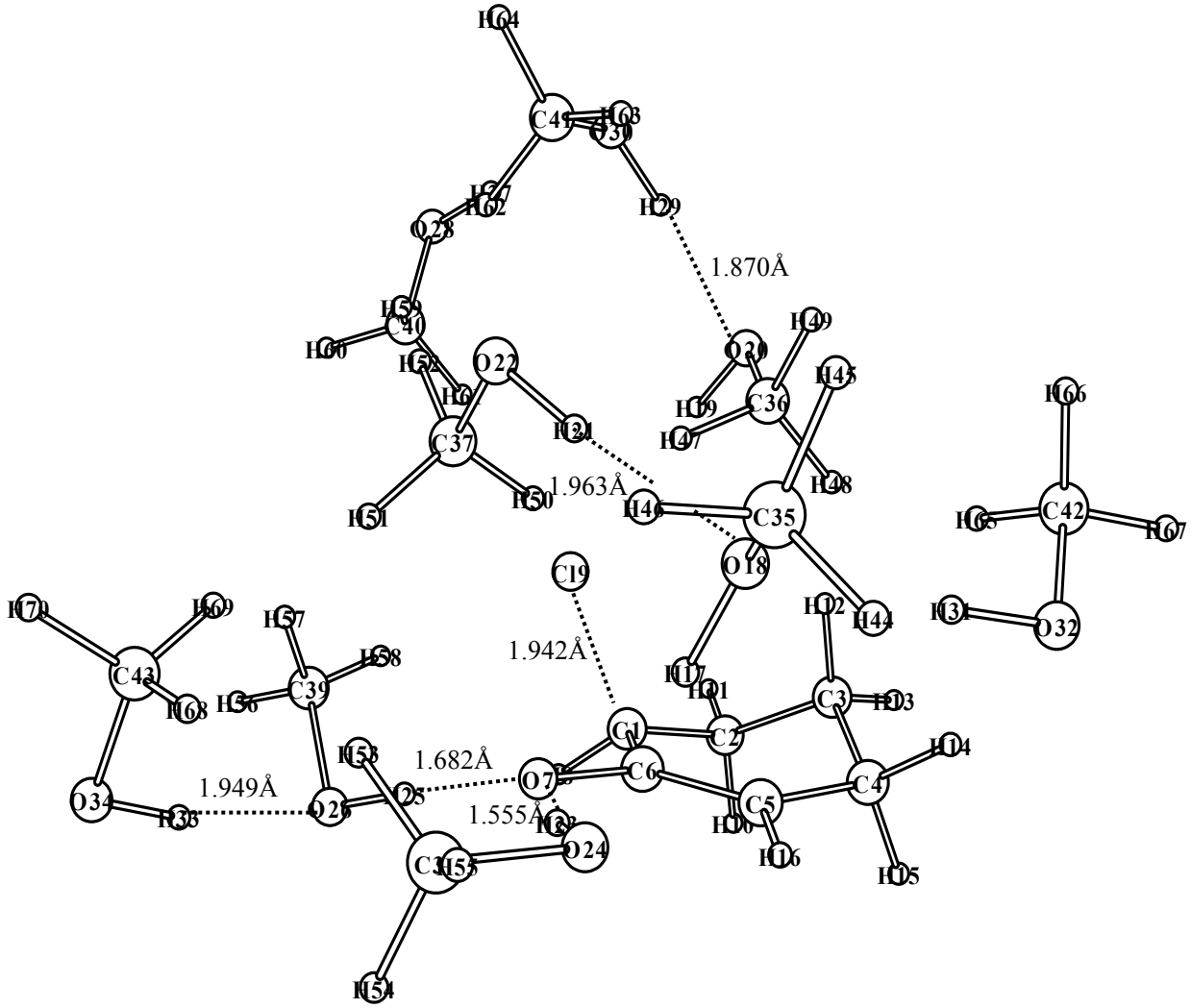
Figure S2. Optimized geometries of precursor, IntA and product and reaction-coordinate vectors for TSs in Figure 1.



precursor'

ΔE= 0 kcal/mol

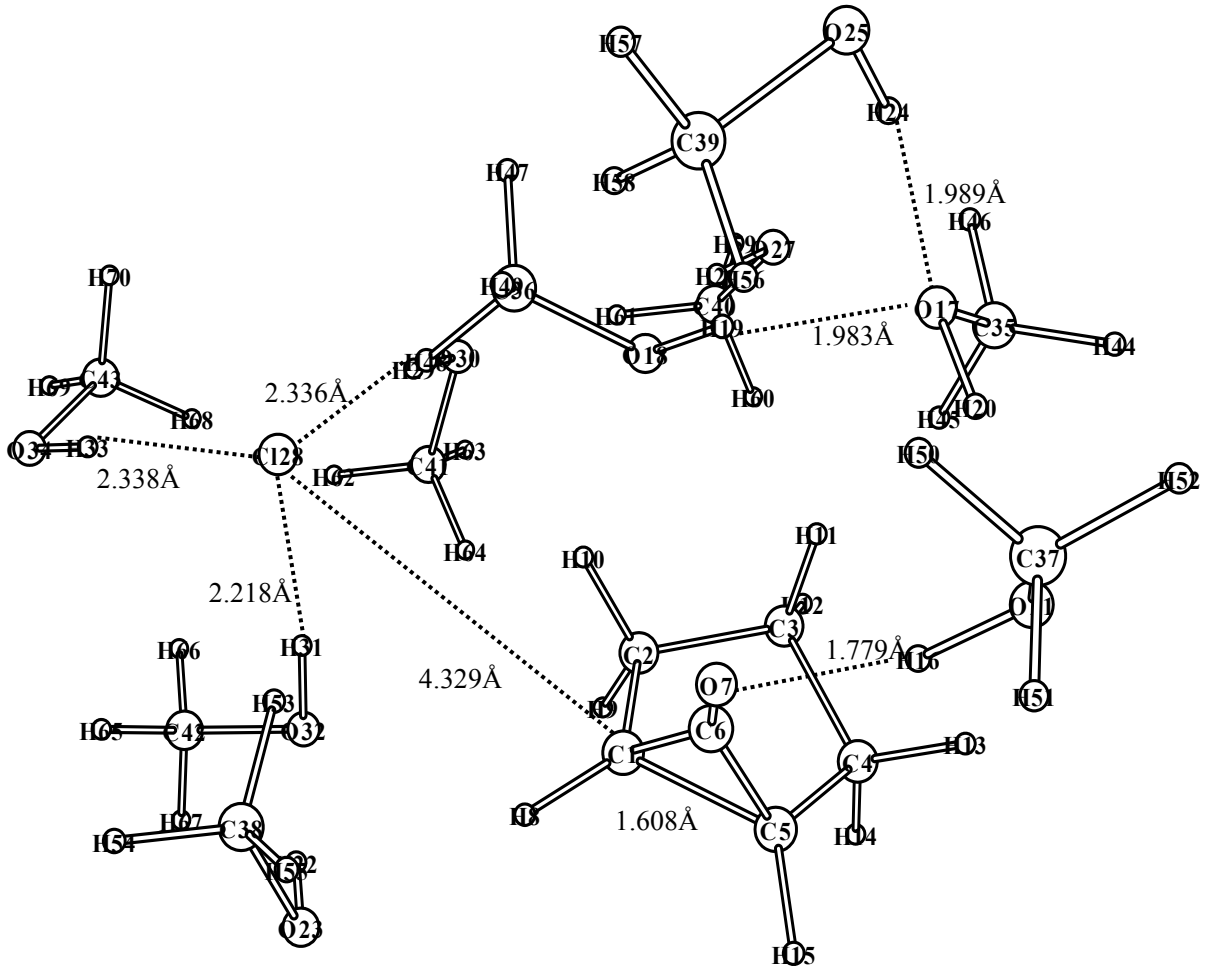
Figure S3-1



Int1B

ΔE= -4.38 kcal/mol

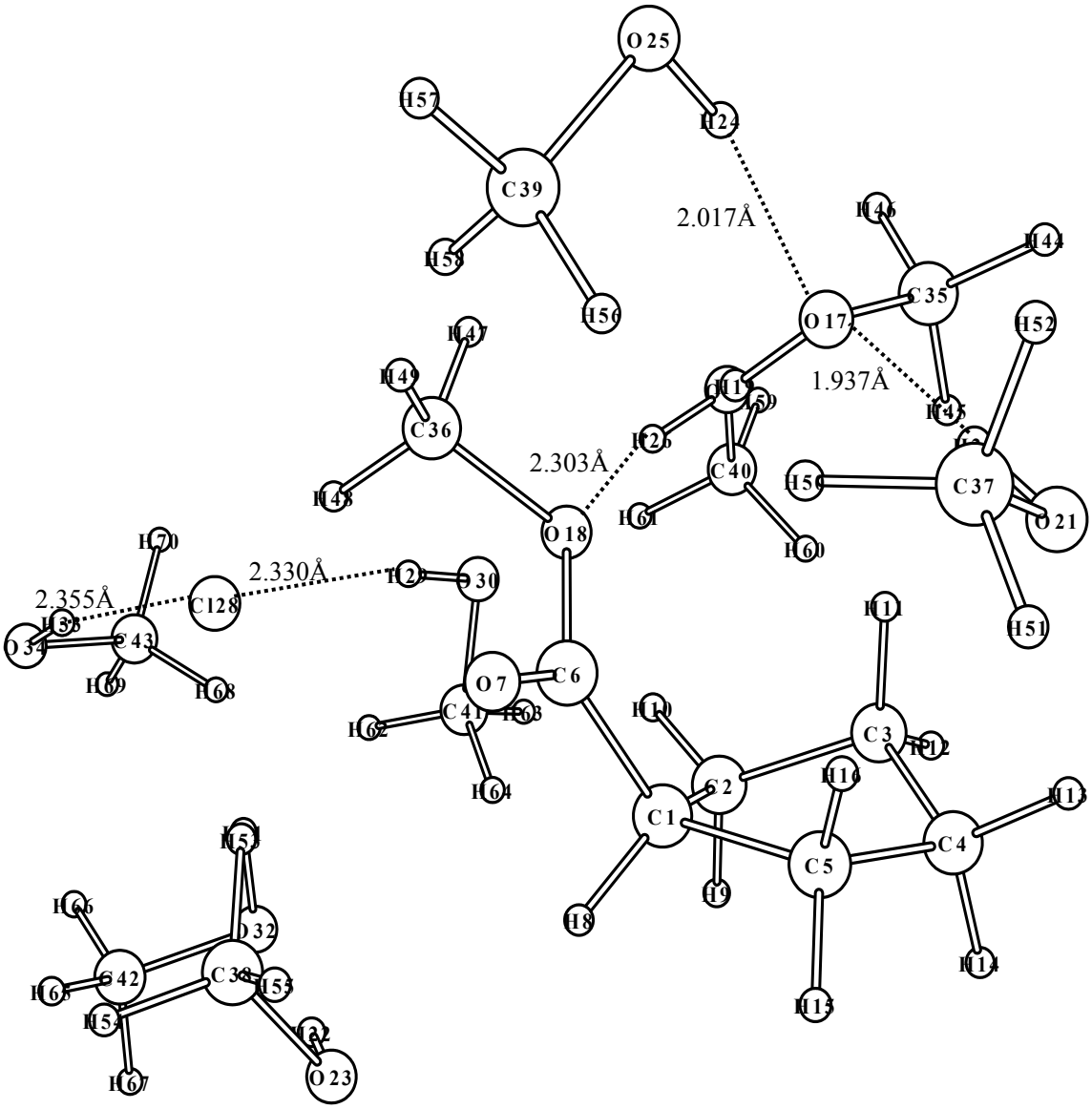
Figure S3-2



Int2B

ΔE= +1.66 kcal/mol

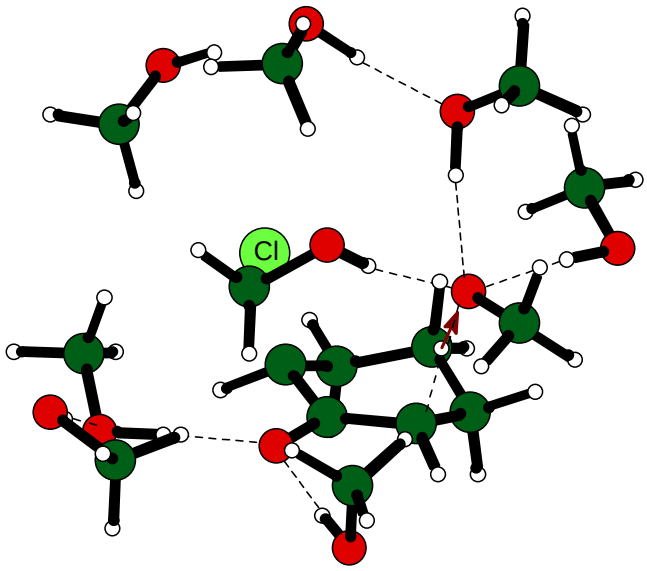
Figure S3-3



product'

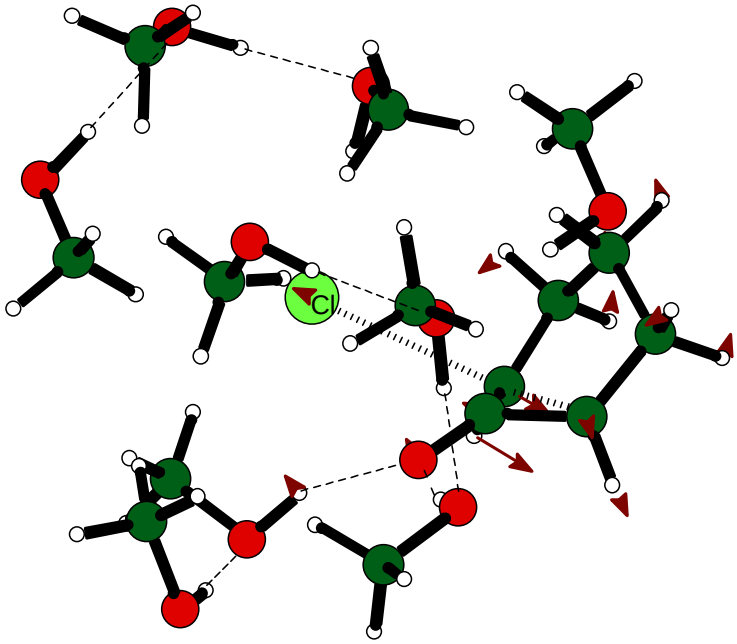
ΔE= -33.96 kcal/mol

Figure S3-4



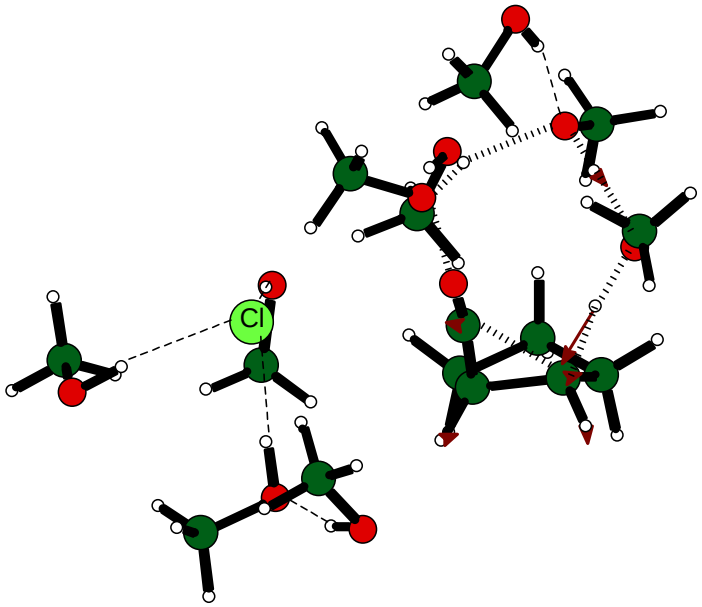
TS1B
$\Delta E^{\ddagger}$ =+1.85 kcal/mol
$\nu^{\ddagger}$ = 1004.73*i* cm^{-1}

Figure S3-5



TS2B
$\Delta E^{\ddagger}$ =+14.15 kcal/mol
$\nu^{\ddagger}$ =231.25*i* cm^{-1}

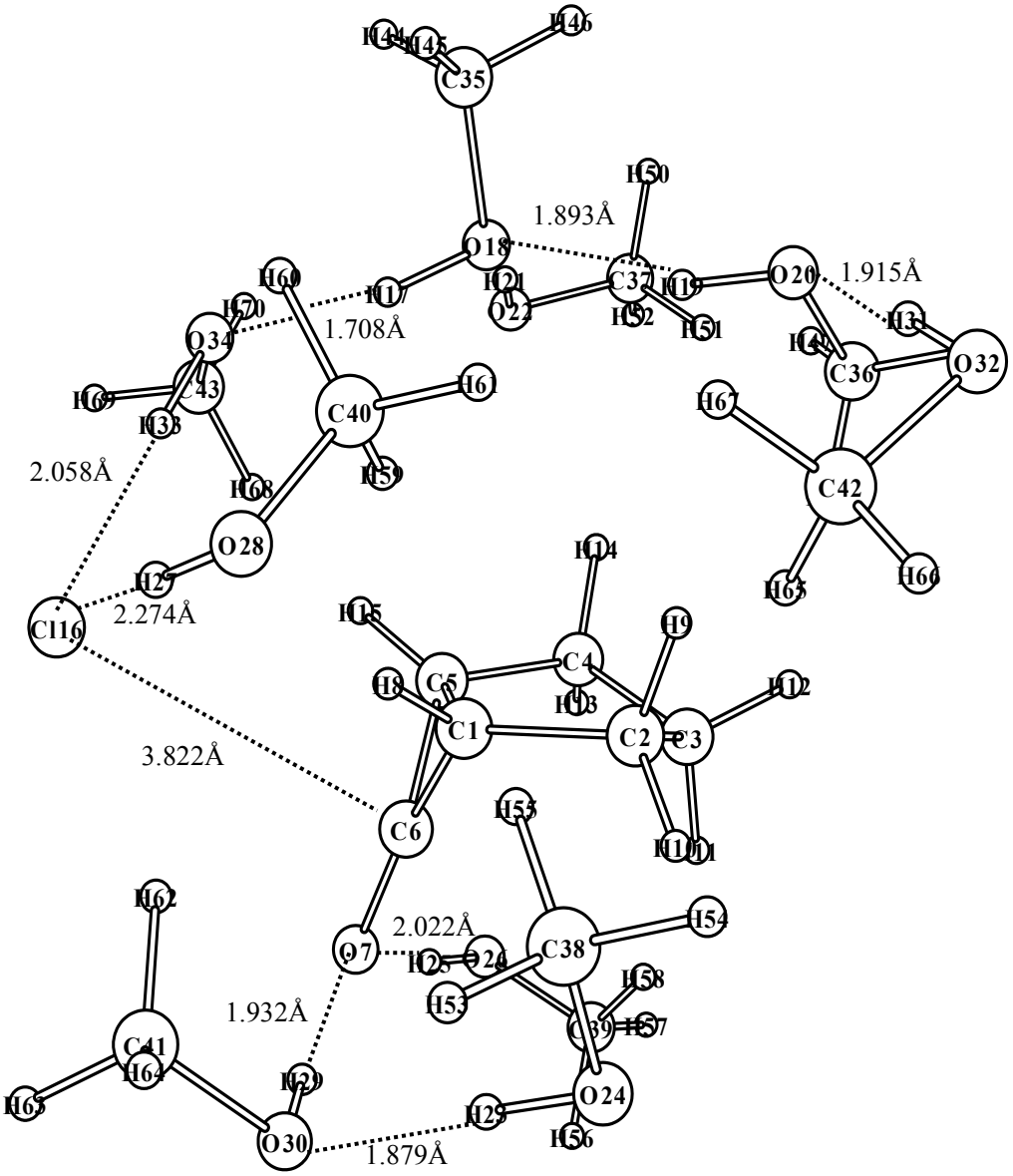
Figure S3-6



TS3B
$\Delta E^{\ddagger}$ =+31.29 kcal/mol
$\nu^{\ddagger}$ = 1160.37*i* cm^{-1}

Figure S3-7

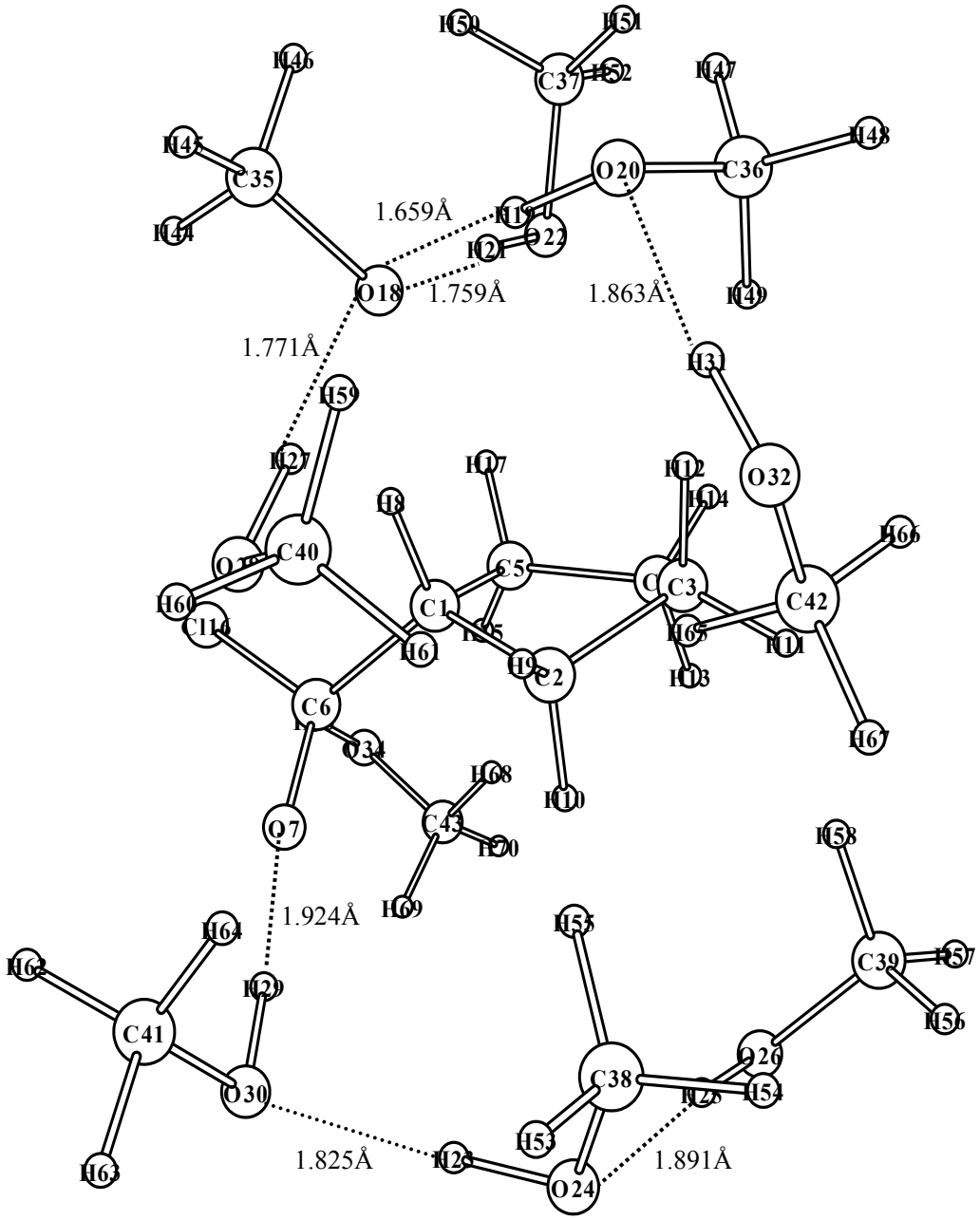
Figure S3. Optimized geometries of precursor, Int1B, Int2B and product' and reaction-coordinate vectors for TSs in Figure 2.



Int2B'

ΔE= -8.18 kcal/mol

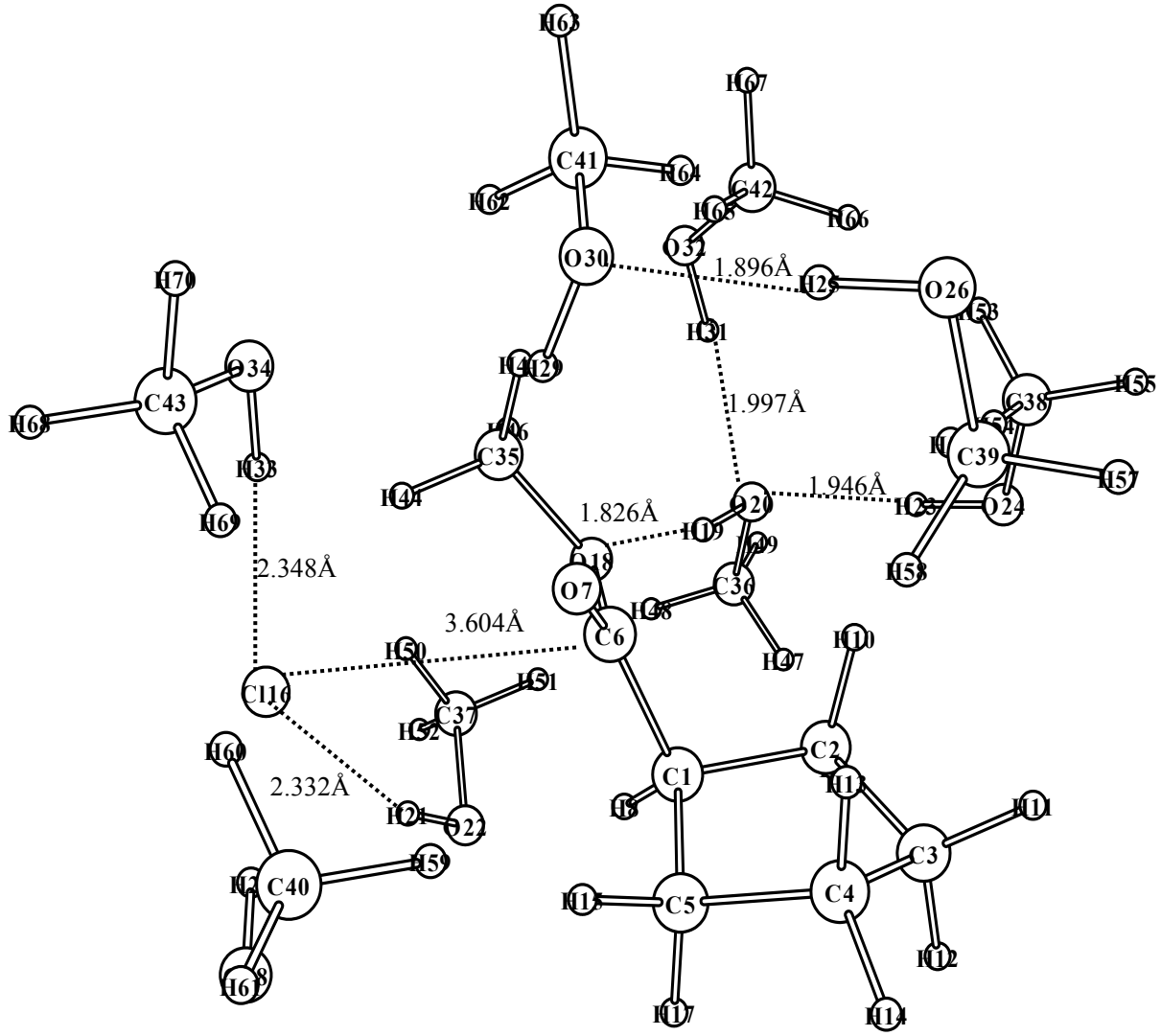
Figure S4-1



Int3B

ΔE= -14.60 kcal/mol

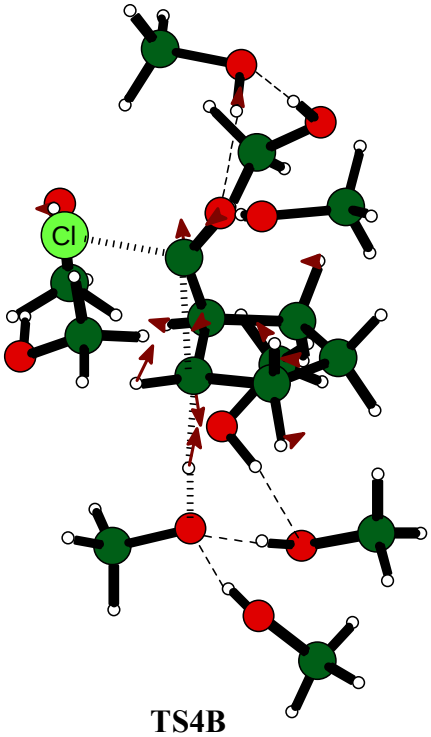
Figure S4-2



product"

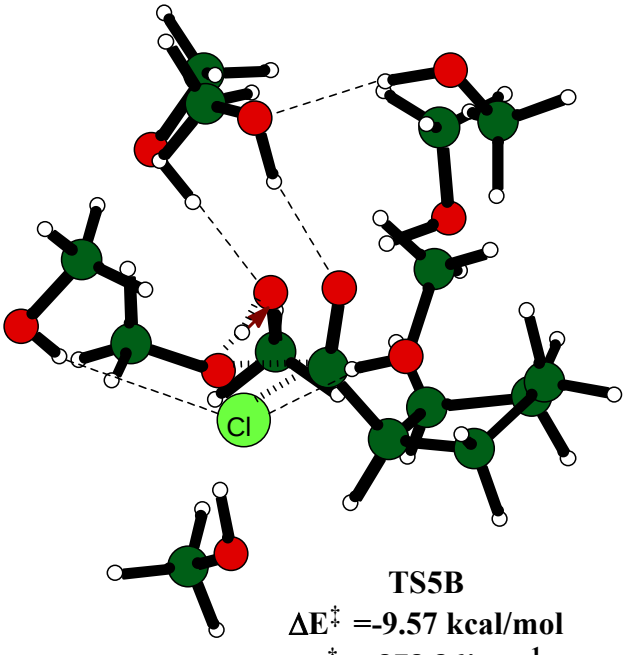
ΔE= -39.25 kcal/mol

Figure S4-3



TS4B
$\Delta E^{\ddagger}$ =+17.75 kcal/mol
$\nu^{\ddagger}$ = 521.89*i* cm^{-1}

Figure S4-4

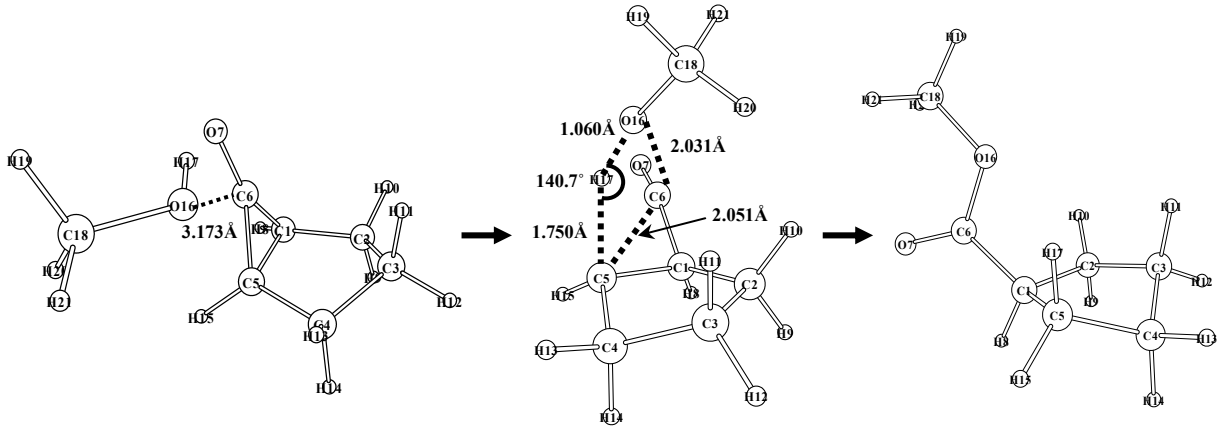


TS5B
$\Delta E^{\ddagger}$ =-9.57 kcal/mol
$\nu^{\ddagger}$ = 878.86*i* cm^{-1}

Figure S4-5

Figure S4. Optimized geometries of Int2B', Int3B and product" and reaction-coordinate vectors for TSs in Figure 4.

bicyclohexanone + $(MeOH)_n$
n = 1



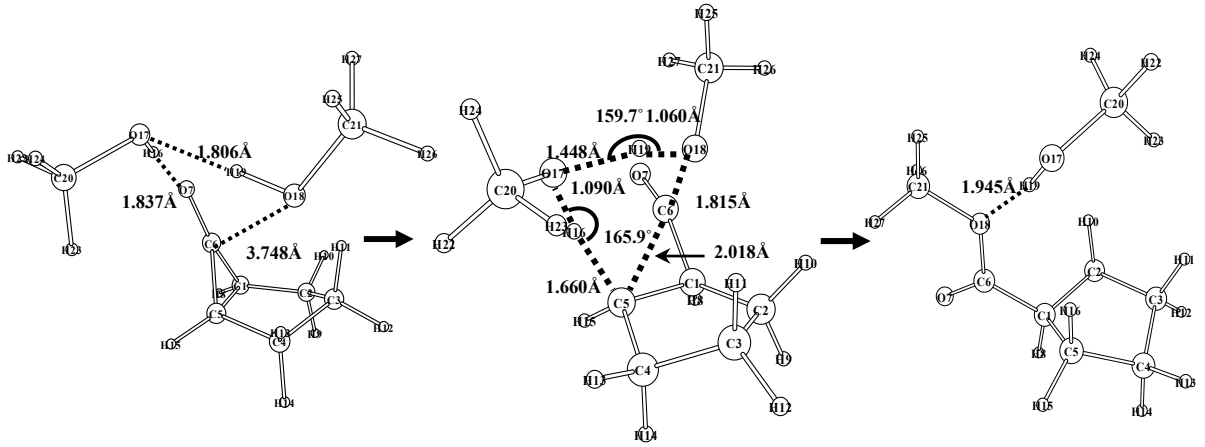
before TS
ΔE = 0 kcal/mol

TS
$\Delta E^{\ddagger}$= 52.63 kcal/mol
$\nu^{\ddagger}$=576.10i cm^{-1}

after TS
ΔE = -53.82 kcal/mol

Figure S5-1

n = 2

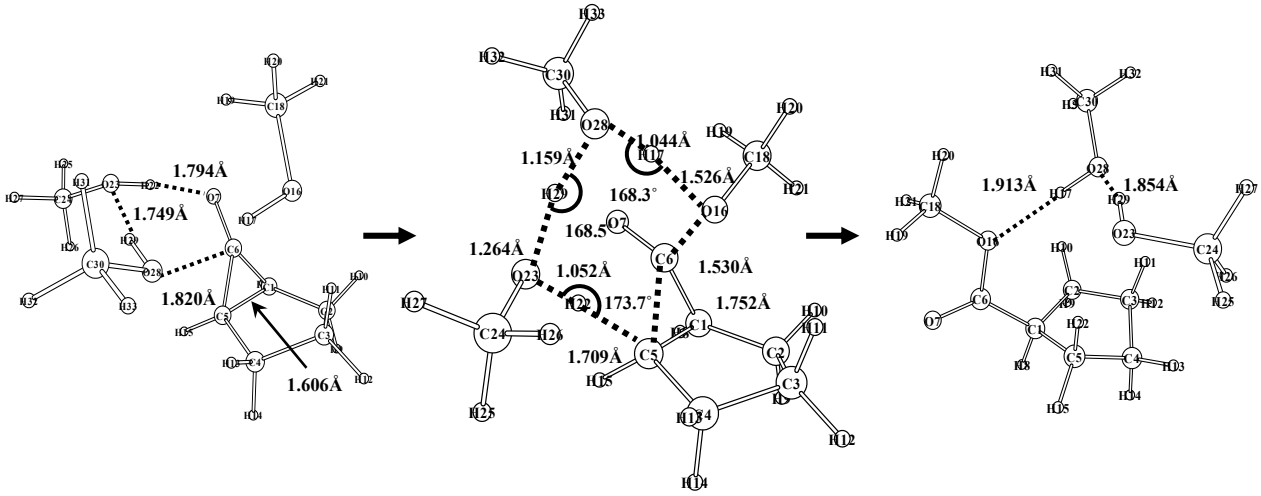


before TS
ΔE = 0 kcal/mol

TS
$\Delta E^{\ddagger}$= 38.67 kcal/mol
$\nu^{\ddagger}$= 533.54i cm^{-1}

after TS
ΔE = -47.64 kcal/mol

Figure S5-2



before TS
ΔE = 0 kcal/mol

TS
$\Delta E^{\ddagger}$= 35.77 kcal/mol
$\nu^{\ddagger}$=537.07í cm^{-1}

after TS
ΔE = -45.60 kcal/mol

Figure S5-3

Figure S5. Optimized geometries of bicyclohexanone + $(MeOH)_n$ (n = 1, 2 and 3) in Scheme 8.

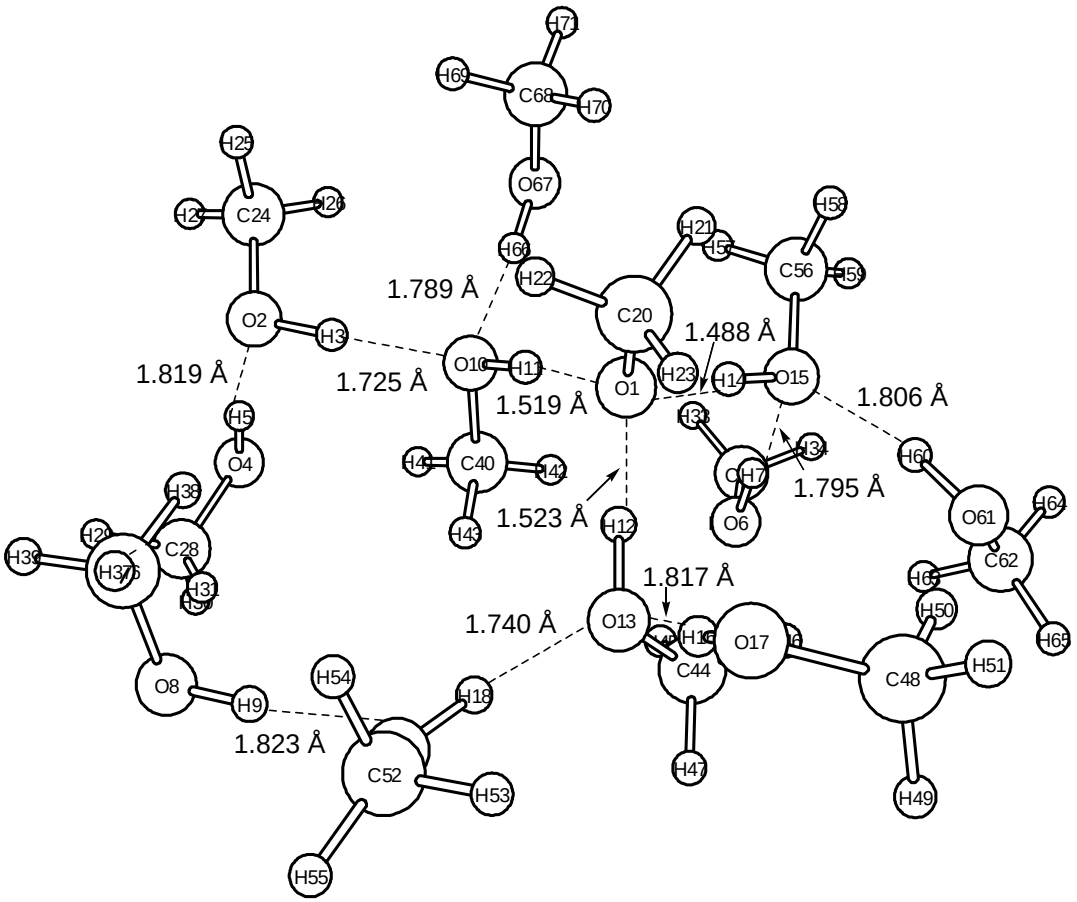


Figure S6. The optimized geometry of $MeO^{-}(MeOH)_{11}$.

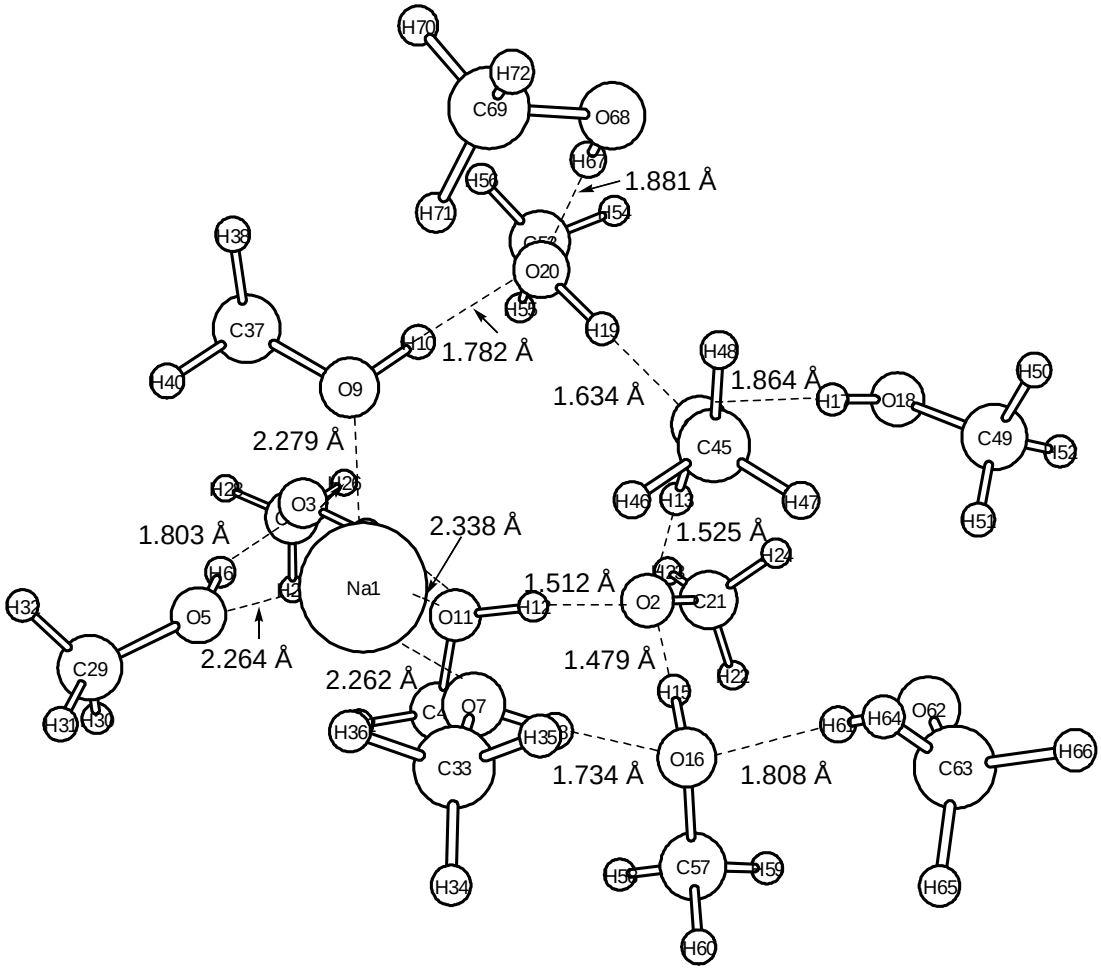
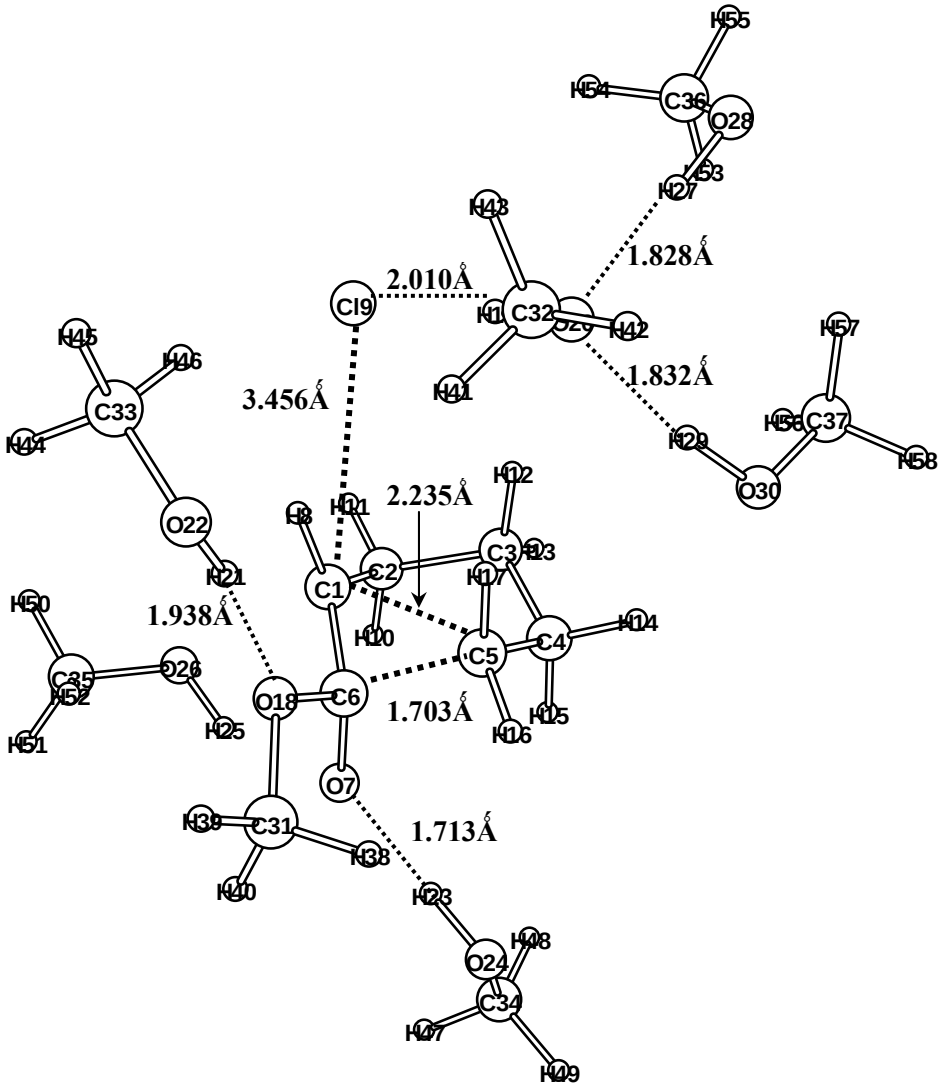
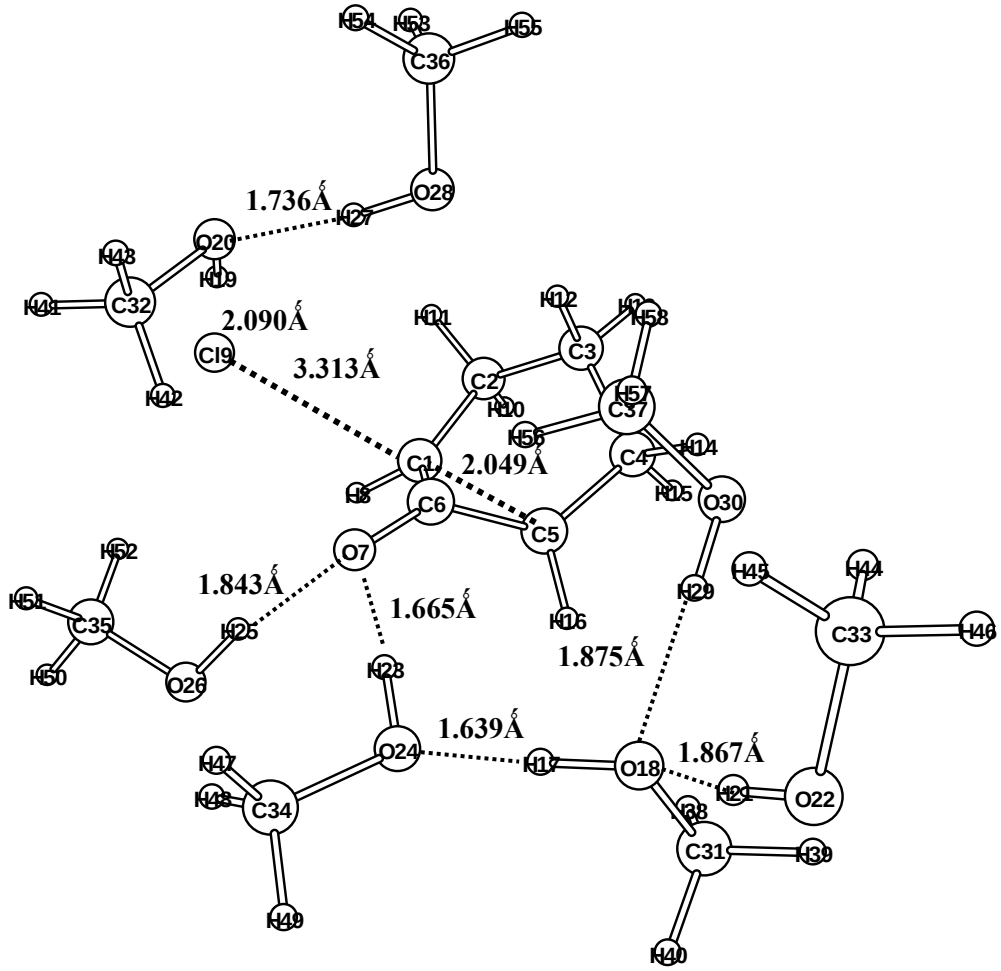


Figure S7. Optimized geometries of $Na^{+}(MeOH)_{11}MeO^{-}$.



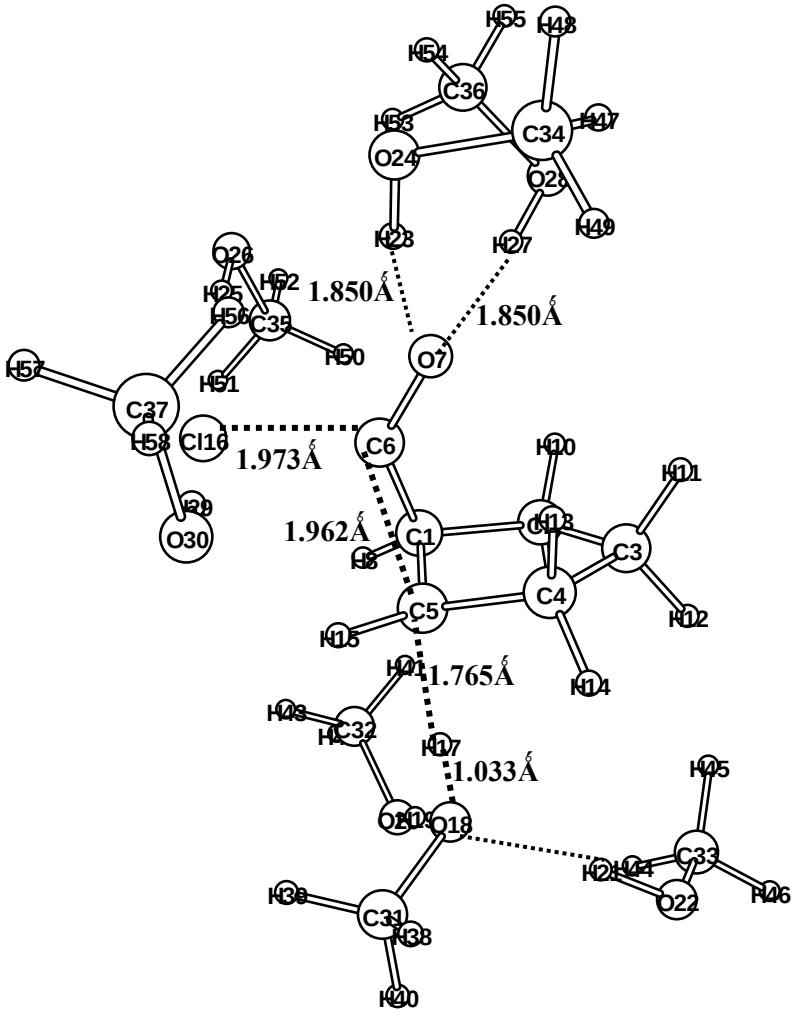
TS2A'

Figure S8-1



TS2B’

Figure S8-2



TS4B'

Figure S8-3

Figure S8. Three TS geomerties, TS2A', TS2B' and TS4B', of a system, α-chlorocyclohexanone + MeO^- and $(MeOH)_6$, which were optimized by RB3LYP/6-31(++)G(d,p).

Cartesian coordinates of Figures 1, 2 and 4
Figure 1 precursor
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625878	0.098677	-0.406837
2	6	0	-2.576312	0.590573	-1.517958
3	6	0	-1.811651	1.009314	-2.785236
4	6	0	-0.856371	-0.084868	-3.292685
5	6	0	0.084706	-0.631454	-2.181303
6	6	0	-0.797698	-1.022973	-1.026929
7	8	0	-1.058838	-2.193694	-0.758683
8	1	0	-2.177984	-0.259898	0.471068
9	17	0	-0.565965	1.452186	0.193203
10	1	0	-3.264139	-0.241325	-1.727045
11	1	0	-3.170101	1.427718	-1.134955
12	1	0	-1.249167	1.932207	-2.564086
13	1	0	-2.531376	1.264150	-3.573818
14	1	0	-0.247678	0.292189	-4.123629
15	1	0	-1.444415	-0.924528	-3.688258
16	1	0	0.626467	-1.514992	-2.528600
17	1	0	0.809684	0.134540	-1.864663
18	8	0	1.580416	-0.969893	0.740842
19	1	0	2.123861	-0.097405	0.574471
20	8	0	2.946247	1.182713	0.229131
21	1	0	0.553841	-1.216674	2.172945
22	8	0	-0.027104	-1.425569	2.949933
23	1	0	-0.174750	-3.557932	-1.810429
24	8	0	0.364944	-4.130597	-2.386443
25	1	0	-2.896169	-2.703601	-0.279470
26	8	0	-3.849178	-2.722873	-0.088949
27	1	0	-1.575122	-0.396673	3.077405
28	8	0	-2.471653	0.005538	3.102689
29	1	0	4.615505	0.972902	0.886808
30	8	0	5.552705	0.765999	1.150214
31	1	0	2.129699	2.631513	0.656724
32	8	0	1.608897	3.454210	0.907244
33	1	0	-2.339783	3.343995	0.323448
34	8	0	-2.936920	3.896121	-0.204552
35	6	0	2.553485	-1.986127	0.707610
36	6	0	3.188009	1.213381	-1.132806
37	6	0	-0.534286	-2.714516	2.673083
38	6	0	1.266407	-4.730734	-1.481584
39	6	0	-3.906784	-2.092173	1.174266
40	6	0	-2.224108	1.384542	3.271279
41	6	0	5.823184	-0.368942	0.363245
42	6	0	1.449889	4.123134	-0.317406
43	6	0	-2.093385	4.316536	-1.258113
44	1	0	3.284673	-1.823529	-0.096350
45	1	0	3.087439	-2.052025	1.663965
46	1	0	2.021949	-2.931896	0.522614
47	1	0	2.262834	1.029526	-1.713950
48	1	0	3.585204	2.192058	-1.439406
49	1	0	3.923605	0.437794	-1.420662
50	1	0	0.182419	-3.335758	2.122793
51	1	0	-0.744223	-3.170695	3.644800
52	1	0	-1.474864	-2.645955	2.098715
53	1	0	1.725467	-3.997494	-0.797330
54	1	0	0.769210	-5.509690	-0.890390
55	1	0	2.041048	-5.189733	-2.101358
56	1	0	-3.651873	-1.022625	1.085040
57	1	0	-4.937325	-2.202061	1.517211
58	1	0	-3.214987	-2.557939	1.895865
59	1	0	-1.635399	1.588360	4.173363
60	1	0	-1.712047	1.811540	2.396739
61	1	0	-3.211576	1.843293	3.372498
62	1	0	5.486341	-1.282678	0.872250
63	1	0	5.328196	-0.309736	-0.620911
64	1	0	6.907996	-0.414481	0.230805
65	1	0	0.773108	3.569426	-0.987669
66	1	0	0.996578	5.092433	-0.083683
67	1	0	2.404033	4.287139	-0.834952
68	1	0	-1.290921	4.973291	-0.896375
69	1	0	-1.644377	3.456029	-1.786865
70	1	0	-2.740836	4.870211	-1.942281

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.00701561 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy: 376.86419 kca/mol

Figure 1 TS1A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.470666	0.016728	-0.323434
2	6	0	-2.503698	0.325609	-1.430215
3	6	0	-1.826906	0.732723	-2.751665
4	6	0	-0.766856	-0.279355	-3.222810
5	6	0	0.262474	-0.630761	-2.111211
6	6	0	-0.558597	-1.051722	-0.920630
7	8	0	-0.821163	-2.234395	-0.692717
8	1	0	-1.947462	-0.342626	0.590908
9	17	0	-0.588241	1.533146	0.164407
10	1	0	-3.104023	-0.586378	-1.553720
11	1	0	-3.173043	1.121453	-1.085603
12	1	0	-1.363482	1.724415	-2.613274
13	1	0	-2.593854	0.853183	-3.527711
14	1	0	-0.234101	0.106736	-4.100921
15	1	0	-1.262079	-1.208133	-3.536640
16	1	0	0.894254	-1.466898	-2.422381
17	1	0	0.895008	0.233570	-1.866250
18	8	0	1.510593	-0.750616	0.726100
19	1	0	2.173091	0.256008	0.505394
20	8	0	2.842693	1.289537	0.279498
21	1	0	0.544473	-0.952770	2.154637
22	8	0	-0.031934	-1.118695	2.956604
23	1	0	0.036008	-3.544186	-1.815868
24	8	0	0.582622	-4.089965	-2.412778
25	1	0	-2.610166	-2.796375	-0.196351
26	8	0	-3.561204	-2.970957	-0.087577
27	1	0	-1.681110	-0.296811	3.015244
28	8	0	-2.623381	-0.012255	2.986646
29	1	0	4.530454	1.049610	1.063990
30	8	0	5.457442	0.830060	1.323255
31	1	0	2.035908	2.873219	0.604795
32	8	0	1.575155	3.738711	0.759828
33	1	0	-2.557452	3.214015	0.180967
34	8	0	-3.155735	3.732541	-0.378705
35	6	0	2.342680	-1.877148	0.667403
36	6	0	3.220243	1.329473	-1.067783
37	6	0	-0.394998	-2.478335	2.853883
38	6	0	1.482613	-4.713714	-1.522170
39	6	0	-3.826173	-2.428289	1.190441
40	6	0	-2.558498	1.393678	3.080237
41	6	0	5.680789	-0.363470	0.608271
42	6	0	1.319613	4.214649	-0.538209
43	6	0	-2.298085	4.129315	-1.429791
44	1	0	3.115971	-1.773624	-0.108653
45	1	0	2.842250	-2.048645	1.630489
46	1	0	1.727394	-2.759512	0.425165
47	1	0	2.354846	1.164282	-1.734766
48	1	0	3.647493	2.315726	-1.284915
49	1	0	3.978112	0.555674	-1.285234
50	1	0	0.430359	-3.101779	2.488823
51	1	0	-0.674434	-2.794391	3.863121
52	1	0	-1.265491	-2.600122	2.185718
53	1	0	1.865709	-4.012304	-0.762095
54	1	0	1.005919	-5.564756	-1.020580
55	1	0	2.307713	-5.077636	-2.139904
56	1	0	-4.066181	-1.360533	1.106875
57	1	0	-4.696247	-2.966559	1.574506
58	1	0	-2.973353	-2.554693	1.877541
59	1	0	-2.062682	1.720416	4.001957
60	1	0	-2.041581	1.832700	2.214121
61	1	0	-3.598602	1.731172	3.089971
62	1	0	5.221724	-1.220422	1.119910
63	1	0	5.274292	-0.303789	-0.415779
64	1	0	6.764392	-0.503321	0.569516
65	1	0	0.627316	3.552207	-1.081501
66	1	0	0.847104	5.194068	-0.412625
67	1	0	2.238461	4.329031	-1.128227
68	1	0	-1.522320	4.823398	-1.079143
69	1	0	-1.812573	3.259405	-1.908092
70	1	0	-2.942200	4.634454	-2.153458

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.00683416 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 374.20544 kca/mol

ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 950.8701i cm-1

Figure 1 IntA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.077508	-1.263707	-0.011323
2	6	0	-0.515367	-2.418543	-0.918774
3	6	0	-1.326441	-1.946290	-2.133874
4	6	0	-0.577421	-0.873226	-2.935309
5	6	0	-0.184300	0.317201	-2.046575
6	6	0	0.658085	-0.171455	-0.847063
7	8	0	1.844240	-0.614036	-1.165575
8	1	0	0.586992	-1.618408	0.786364
9	17	0	-1.579527	-0.648842	0.924977
10	1	0	0.407657	-2.913824	-1.243684
11	1	0	-1.091469	-3.145774	-0.335739
12	1	0	-2.301423	-1.543362	-1.782474
13	1	0	-1.557733	-2.809458	-2.772373
14	1	0	-1.191699	-0.526046	-3.777757
15	1	0	0.337050	-1.305360	-3.359090
16	1	0	0.436458	1.019742	-2.617801
17	1	0	-1.086312	0.855264	-1.708339
18	8	0	0.725760	1.083378	0.180464
19	1	0	-0.887527	2.080765	0.446610
20	8	0	-1.658993	2.700115	0.467487
21	1	0	1.899498	0.550039	1.580118
22	8	0	2.509614	0.384660	2.334132
23	1	0	2.680189	0.186654	-2.497071
24	8	0	3.148323	0.731001	-3.179974
25	1	0	2.574459	-2.230654	-0.901700
26	8	0	2.887303	-3.157930	-0.784126
27	1	0	1.824004	-1.179091	3.124287
28	8	0	1.473374	-2.046650	3.417268
29	1	0	-1.276489	4.337220	1.585476
30	8	0	-0.988709	5.222339	1.878082
31	1	0	-3.432154	1.694570	0.154923
32	8	0	-4.300733	1.371554	-0.146642
33	1	0	-3.025284	-2.735699	1.134192
34	8	0	-3.565085	-3.490639	0.854117
35	6	0	1.565072	2.120393	-0.298967
36	6	0	-1.629326	3.323664	-0.803107
37	6	0	3.702396	-0.061013	1.716083
38	6	0	4.290975	1.166410	-2.483178
39	6	0	2.704756	-3.363144	0.598392
40	6	0	0.176858	-1.741142	3.880912
41	6	0	0.270325	5.354746	1.254571
42	6	0	-3.985784	0.585673	-1.274978
43	6	0	-4.254573	-2.968293	-0.262553
44	1	0	1.123599	2.611989	-1.176359
45	1	0	1.624626	2.840585	0.525337
46	1	0	2.575076	1.762417	-0.558440
47	1	0	-1.522418	2.576852	-1.607869
48	1	0	-2.584299	3.846590	-0.899157
49	1	0	-0.801461	4.051236	-0.856977
50	1	0	3.975915	0.559736	0.852747
51	1	0	4.475376	0.017362	2.485268
52	1	0	3.610373	-1.111537	1.391654
53	1	0	4.031192	1.578400	-1.492980
54	1	0	5.014555	0.352466	-2.349500
55	1	0	4.744942	1.951306	-3.094894
56	1	0	1.714782	-3.009816	0.937142
57	1	0	2.794037	-4.438794	0.766977
58	1	0	3.478038	-2.834630	1.179647
59	1	0	0.201646	-1.051652	4.733817
60	1	0	-0.451318	-1.314989	3.085263
61	1	0	-0.245001	-2.696517	4.204777
62	1	0	1.034137	4.758391	1.769987
63	1	0	0.230207	5.049298	0.194846
64	1	0	0.527028	6.414477	1.324942
65	1	0	-3.248686	-0.211048	-1.055287
66	1	0	-4.930674	0.126283	-1.577962
67	1	0	-3.599296	1.204165	-2.096533
68	1	0	-4.984464	-2.204180	0.033937
69	1	0	-3.561741	-2.532365	-1.004753
70	1	0	-4.777659	-3.820279	-0.703557

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.01167167 a.u.

ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 378.71676 kca/mol

Figure 1 TS2A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.079352	-1.638692	-0.251545
2	6	0	0.831728	-2.905802	-0.130256
3	6	0	2.037537	-2.675801	0.840147
4	6	0	1.555504	-1.946012	2.094619
5	6	0	0.772337	-0.712091	1.681036
6	6	0	-0.662926	-1.136738	0.897162
7	8	0	-1.399561	-1.955959	1.591454
8	1	0	0.342570	-0.934160	-1.052772
9	17	0	2.115291	0.720231	-1.778964
10	1	0	0.179963	-3.670599	0.300920
11	1	0	1.213874	-3.211346	-1.106740
12	1	0	2.800024	-2.079829	0.311823
13	1	0	2.483388	-3.650477	1.070673
14	1	0	2.414160	-1.645681	2.711278
15	1	0	0.915692	-2.594097	2.702345
16	1	0	0.319167	-0.171914	2.528741
17	1	0	1.391795	-0.004829	1.098621
18	8	0	-1.272027	0.147483	0.476810
19	1	0	1.986095	2.487623	-0.487550
20	8	0	2.099914	3.257089	0.121646
21	1	0	-1.755743	0.748598	-1.247985
22	8	0	-2.005809	1.059352	-2.139648
23	1	0	-1.618158	-1.515499	3.297493
24	8	0	-1.766937	-1.196548	4.220920
25	1	0	-2.032638	-2.663076	0.075676
26	8	0	-1.883720	-2.827982	-0.893959
27	1	0	-3.742324	0.571388	-2.618241
28	8	0	-4.647366	0.264678	-2.845912
29	1	0	0.510601	4.509746	-0.204727
30	8	0	-0.273650	5.089932	-0.166895
31	1	0	4.162299	2.358697	0.570751
32	8	0	4.759292	1.727177	1.004440
33	1	0	2.789363	-1.309218	-2.511204
34	8	0	3.106508	-2.228265	-2.637856
35	6	0	-1.754629	0.963759	1.532011
36	6	0	1.740787	2.715918	1.378202
37	6	0	-1.077337	0.380624	-2.969657
38	6	0	-3.130487	-0.845919	4.221507
39	6	0	-2.944220	-2.162288	-1.553361
40	6	0	-5.435428	0.782596	-1.798664
41	6	0	-1.146836	4.400894	0.698968
42	6	0	4.204757	0.488127	0.603958
43	6	0	4.314226	-2.219864	-1.910380
44	1	0	-0.998341	1.070108	2.325350
45	1	0	-1.929221	1.928601	1.033351
46	1	0	-2.681832	0.560335	1.964560
47	1	0	1.932891	1.626948	1.424065
48	1	0	2.347871	3.232639	2.126935
49	1	0	0.674110	2.902535	1.590553
50	1	0	-1.519924	-0.578469	-3.285927
51	1	0	-0.921117	1.022180	-3.839097
52	1	0	-0.114974	0.194631	-2.455042
53	1	0	-3.367270	-0.136870	3.410508
54	1	0	-3.776118	-1.727390	4.124380
55	1	0	-3.317752	-0.367821	5.186924
56	1	0	-2.533181	-1.797915	-2.506995
57	1	0	-3.753937	-2.873886	-1.744802
58	1	0	-3.332986	-1.311315	-0.978800
59	1	0	-5.109421	0.405816	-0.820141
60	1	0	-5.425754	1.879417	-1.783536
61	1	0	-6.452203	0.433920	-1.999070
62	1	0	-1.563653	3.484897	0.244559
63	1	0	-0.643364	4.107471	1.635679
64	1	0	-1.957450	5.100331	0.915796
65	1	0	3.141856	0.397262	0.915891
66	1	0	4.255686	0.343908	-0.486734
67	1	0	4.795891	-0.278701	1.111870
68	1	0	4.992258	-1.423766	-2.241172
69	1	0	4.120404	-2.098085	-0.829731
70	1	0	4.778100	-3.193954	-2.086569

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1810.95264493 a.u.

ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 376.53762 kca/mol
ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 361.2689ί cm-1

Figure 1 product
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075392	-1.522459	-1.082051
2	6	0	0.247140	-3.018266	-1.206135
3	6	0	-1.150674	-3.651143	-1.170907
4	6	0	-2.014603	-2.711319	-2.046050
5	6	0	-1.337781	-1.311128	-1.969233
6	6	0	1.075777	-0.598657	-1.382073
7	8	0	2.224674	-0.955908	-1.600208
8	1	0	-0.362139	-1.295487	-0.045787
9	17	0	-2.005154	0.295779	1.684212
10	1	0	0.737357	-3.215518	-2.169413
11	1	0	0.920807	-3.376843	-0.422801
12	1	0	-1.524845	-3.646666	-0.134034
13	1	0	-1.161014	-4.688549	-1.523383
14	1	0	-3.055179	-2.673925	-1.699219
15	1	0	-2.036142	-3.065042	-3.083878
16	1	0	-1.058502	-0.957366	-2.968582
17	1	0	-2.001403	-0.550258	-1.524117
18	8	0	0.670630	0.701814	-1.375037
19	1	0	-2.607958	2.003372	0.505624
20	8	0	-2.998804	2.675187	-0.105522
21	1	0	0.195992	0.453495	1.676272
22	8	0	1.136650	0.181431	1.766581
23	1	0	3.988027	-0.007095	-1.835252
24	8	0	4.819691	0.493287	-1.780498
25	1	0	3.158242	-2.564764	-0.819925
26	8	0	3.612715	-3.262876	-0.320037
27	1	0	2.275893	1.508220	2.502255
28	8	0	2.911384	2.213803	2.739564
29	1	0	-1.886151	4.337472	0.060413
30	8	0	-1.304085	5.118215	-0.016440
31	1	0	-4.802992	1.456546	-0.189325
32	8	0	-5.391262	0.727568	-0.449589
33	1	0	-1.693361	-1.972875	2.487057
34	8	0	-1.943360	-2.914605	2.562068
35	6	0	1.685937	1.710886	-1.477360
36	6	0	-2.616148	2.191058	-1.379601
37	6	0	0.986480	-0.895407	2.673988
38	6	0	4.930735	0.748219	-0.395781
39	6	0	3.881052	-2.643485	0.919841
40	6	0	2.818512	3.089194	1.638711
41	6	0	-0.343809	4.708740	-0.962780
42	6	0	-4.544864	-0.396460	-0.301894
43	6	0	-3.142356	-2.904348	1.814760
44	1	0	2.171329	1.689679	-2.457700
45	1	0	1.108102	2.636494	-1.339223
46	1	0	2.445448	1.629337	-0.674721
47	1	0	-2.573548	1.085051	-1.403506
48	1	0	-3.374123	2.546437	-2.083613
49	1	0	-1.636316	2.606163	-1.668624
50	1	0	1.655145	-1.698061	2.332596
51	1	0	1.284474	-0.574046	3.677530
52	1	0	-0.059551	-1.240403	2.682291
53	1	0	4.088204	1.373060	-0.039385
54	1	0	4.963039	-0.183635	0.192419
55	1	0	5.868878	1.293592	-0.271719
56	1	0	2.952879	-2.411918	1.468786
57	1	0	4.465998	-3.372270	1.486241
58	1	0	4.467545	-1.717648	0.797331
59	1	0	3.062954	2.572323	0.689084
60	1	0	1.820043	3.537007	1.547984
61	1	0	3.555192	3.874835	1.823630
62	1	0	0.412836	4.038198	-0.517655
63	1	0	-0.804359	4.179580	-1.813649
64	1	0	0.143062	5.623066	-1.309937
65	1	0	-3.613383	-0.280247	-0.893468
66	1	0	-4.256945	-0.577138	0.750367
67	1	0	-5.113963	-1.247305	-0.685335
68	1	0	-3.497000	-1.875245	1.630630
69	1	0	-2.951614	-3.401870	0.850155
70	1	0	-3.889221	-3.473891	2.374294

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.05596035 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 379.75116 kca/mol

Figure 2 precursor
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.138708	1.929830	-1.720508
2	6	0	0.473541	3.204022	-2.243819
3	6	0	-0.763945	3.591645	-1.428959
4	6	0	-0.427101	3.769937	0.056260
5	6	0	0.269153	2.527255	0.654195
6	6	0	1.351168	1.960952	-0.203136
7	8	0	2.400156	1.501118	0.257091
8	1	0	2.107302	1.735700	-2.199200
9	17	0	0.138848	0.445623	-2.112662
10	1	0	1.225084	4.007096	-2.177445
11	1	0	0.238445	3.074647	-3.306467
12	1	0	-1.546752	2.824746	-1.528439
13	1	0	-1.184546	4.523160	-1.828606
14	1	0	-1.353004	3.948064	0.609618
15	1	0	0.220205	4.651104	0.183510
16	1	0	0.692637	2.721656	1.646649
17	1	0	-0.491434	1.719336	0.808834
18	8	0	-1.937723	0.456140	1.431274
19	1	0	-3.172863	-0.607622	1.034213
20	8	0	-3.890458	-1.247724	0.722144
21	1	0	-0.923898	-1.028992	1.452709
22	8	0	-0.448554	-1.900978	1.511000
23	1	0	2.649074	1.569673	2.208879
24	8	0	2.655166	1.585262	3.181747
25	1	0	3.546875	0.339979	-0.679281
26	8	0	4.103281	-0.272431	-1.201356
27	1	0	-1.596020	-2.544855	-2.325450
28	8	0	-0.969144	-2.346422	-3.056004
29	1	0	-3.135474	-2.464625	-0.410409
30	8	0	-2.763393	-3.177080	-0.984887
31	1	0	-2.990345	1.742963	0.738337
32	8	0	-3.542664	2.468966	0.345051
33	1	0	4.419018	-1.731226	0.028287
34	8	0	4.545795	-2.440907	0.687982
35	6	0	-1.959375	0.749693	2.786526
36	6	0	-4.216448	-1.987331	1.876653
37	6	0	0.759196	-1.667932	0.823393
38	6	0	1.839567	0.475786	3.505249
39	6	0	3.226442	-0.728919	-2.211763
40	6	0	0.232217	-2.932709	-2.603265
41	6	0	-1.906646	-3.869211	-0.093584
42	6	0	-3.910644	1.927803	-0.901889
43	6	0	4.258379	-1.807111	1.915683
44	1	0	-2.459249	1.708838	2.987751
45	1	0	-2.483743	-0.029749	3.361650
46	1	0	-0.928426	0.823658	3.182846
47	1	0	-3.376388	-2.619768	2.195585
48	1	0	-4.510250	-1.335458	2.708891
49	1	0	-5.062317	-2.624146	1.600799
50	1	0	0.644700	-0.957508	-0.008889
51	1	0	1.530855	-1.286254	1.520625
52	1	0	1.087500	-2.633882	0.423797
53	1	0	2.130510	-0.426816	2.932132
54	1	0	1.995078	0.298730	4.571850
55	1	0	0.772537	0.692766	3.318399
56	1	0	2.786371	0.123803	-2.756588
57	1	0	3.843520	-1.326112	-2.886323
58	1	0	2.402704	-1.348874	-1.811197
59	1	0	0.053000	-3.717428	-1.850921
60	1	0	0.725571	-3.363970	-3.478682
61	1	0	0.886589	-2.156490	-2.166314
62	1	0	-1.149681	-4.358258	-0.723758
63	1	0	-1.402172	-3.189287	0.625250
64	1	0	-2.472555	-4.633846	0.450374
65	1	0	-3.058463	1.965122	-1.601694
66	1	0	-4.269269	0.894585	-0.822685
67	1	0	-4.712535	2.563933	-1.288066
68	1	0	4.945942	-0.976517	2.116579
69	1	0	3.215378	-1.432021	1.964417
70	1	0	4.395108	-2.581265	2.675136

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.00314793 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 378.41800 kca/mol

Figure 2 TS1B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.260708	-1.475103	-2.142171
2	6	0	0.831630	-2.145408	-2.970101
3	6	0	2.130795	-2.321261	-2.181814
4	6	0	1.892283	-3.147059	-0.910459
5	6	0	0.704074	-2.633880	-0.098450
6	6	0	-0.423446	-2.062998	-0.731382
7	8	0	-1.565493	-1.936580	-0.196372
8	1	0	-1.235604	-1.524087	-2.643446
9	17	0	0.042489	0.348138	-2.020229
10	1	0	0.447167	-3.138376	-3.253349
11	1	0	0.989576	-1.586787	-3.899863
12	1	0	2.538749	-1.333243	-1.911559
13	1	0	2.884739	-2.809500	-2.813674
14	1	0	2.804520	-3.124810	-0.301597
15	1	0	1.734600	-4.201768	-1.196750
16	1	0	0.434791	-3.234933	0.775143
17	1	0	1.256766	-1.474436	0.662194
18	8	0	1.797174	-0.632901	1.295193
19	1	0	2.458373	1.033923	0.846299
20	8	0	2.929255	1.873023	0.639609
21	1	0	0.275665	0.631458	1.660999
22	8	0	-0.343909	1.324583	1.960853
23	1	0	-1.819603	-2.758533	1.432685
24	8	0	-1.916862	-3.130548	2.336200
25	1	0	-2.965864	-1.167908	-0.941931
26	8	0	-3.776051	-0.799370	-1.375946
27	1	0	0.276027	3.861122	-1.457786
28	8	0	-0.317879	3.785570	-2.232870
29	1	0	1.821262	3.312970	0.308875
30	8	0	1.291861	4.124347	0.149040
31	1	0	3.684896	-1.057034	0.833564
32	8	0	4.593978	-1.336960	0.607269
33	1	0	-4.714736	0.111748	-0.009152
34	8	0	-5.156022	0.560254	0.742528
35	6	0	1.909649	-1.023846	2.647455
36	6	0	3.631867	2.166759	1.828981
37	6	0	-1.519053	1.052709	1.220020
38	6	0	-1.780221	-1.984013	3.145272
39	6	0	-3.264084	0.168822	-2.265958
40	6	0	-1.557776	3.462339	-1.640360
41	6	0	0.322721	4.068602	1.181523
42	6	0	4.860241	-0.599642	-0.566338
43	6	0	-4.828506	-0.264366	1.839677
44	1	0	2.521938	-1.927834	2.750767
45	1	0	2.393208	-0.192717	3.172813
46	1	0	0.919385	-1.216454	3.090899
47	1	0	2.949252	2.309383	2.676556
48	1	0	4.350593	1.373612	2.071042
49	1	0	4.166953	3.098724	1.627978
50	1	0	-1.300847	0.781496	0.175933
51	1	0	-2.101281	0.239759	1.697108
52	1	0	-2.103831	1.977946	1.240178
53	1	0	-2.381229	-1.134347	2.765397
54	1	0	-2.136238	-2.268899	4.138461
55	1	0	-0.725380	-1.668681	3.211864
56	1	0	-2.519711	-0.282770	-2.943516
57	1	0	-4.120558	0.530425	-2.839202
58	1	0	-2.785197	1.012693	-1.737142
59	1	0	-1.639326	3.856892	-0.614312
60	1	0	-2.330183	3.909549	-2.271569
61	1	0	-1.697379	2.366462	-1.617926
62	1	0	-0.626603	4.403467	0.736873
63	1	0	0.188175	3.047128	1.591065
64	1	0	0.611755	4.758390	1.981030
65	1	0	4.079059	-0.757225	-1.329139
66	1	0	4.949361	0.473086	-0.352230
67	1	0	5.815908	-0.976152	-0.940297
68	1	0	-5.239101	-1.274931	1.726746
69	1	0	-3.732743	-0.334048	1.995084
70	1	0	-5.284834	0.215616	2.709397

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1810.99522013 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 375.2955 kca/mol
ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 1004.7264í cm-1

Figure 2 Int1B
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.239799	0.291201	2.741718
2	6	0	1.052740	-0.582836	3.688769
3	6	0	2.207828	-1.277381	2.963592
4	6	0	3.135527	-0.218645	2.360330
5	6	0	2.362966	0.831874	1.608488
6	6	0	1.017084	1.045556	1.694063
7	8	0	0.332873	1.909028	0.978486
8	1	0	-0.429758	0.975821	3.265906
9	17	0	-1.101813	-0.829769	1.895325
10	1	0	1.466840	0.083552	4.462183
11	1	0	0.396836	-1.293279	4.203379
12	1	0	1.810835	-1.916728	2.154991
13	1	0	2.751928	-1.933112	3.656001
14	1	0	3.861730	-0.685087	1.678675
15	1	0	3.738962	0.233409	3.170659
16	1	0	2.934137	1.479530	0.948013
17	1	0	2.102900	1.435223	-1.709720
18	8	0	2.239606	0.539284	-2.145792
19	1	0	-0.428448	-3.017391	1.006152
20	8	0	0.037695	-3.514217	0.314074
21	1	0	0.342945	0.155932	-2.476219
22	8	0	-0.583211	-0.033922	-2.718008
23	1	0	1.191689	2.564370	-0.140137
24	8	0	1.816356	2.873232	-0.900463
25	1	0	-1.131373	2.566019	1.482655
26	8	0	-1.979823	3.002594	1.788517
27	1	0	-3.564123	-3.702448	-0.632806
28	8	0	-4.326522	-3.294384	-0.176474
29	1	0	-1.234844	-3.957382	-0.982167
30	8	0	-1.951060	-4.193537	-1.611686
31	1	0	3.796227	-0.298073	-1.334608
32	8	0	4.623462	-0.729658	-1.038778
33	1	0	-2.520027	4.167249	0.321916
34	8	0	-2.889642	4.580327	-0.486405
35	6	0	2.710356	0.841824	-3.443296
36	6	0	0.852551	-2.497736	-0.248866
37	6	0	-1.276067	0.159661	-1.500056
38	6	0	1.070153	3.779029	-1.680738
39	6	0	-2.967896	2.019055	1.565307
40	6	0	-3.886816	-1.969960	0.041211
41	6	0	-1.927989	-3.146019	-2.564184
42	6	0	4.235837	-2.065963	-0.818234
43	6	0	-2.617987	3.607850	-1.473146
44	1	0	3.709344	1.293235	-3.409751
45	1	0	2.761034	-0.116591	-3.967424
46	1	0	2.027721	1.515944	-3.975795
47	1	0	0.289116	-1.561414	-0.408920
48	1	0	1.719868	-2.288611	0.408850
49	1	0	1.203446	-2.893525	-1.206194
50	1	0	-0.670285	-0.111230	-0.617437
51	1	0	-1.618766	1.203655	-1.403567
52	1	0	-2.152097	-0.511543	-1.549345
53	1	0	0.072138	3.388544	-1.940907
54	1	0	0.951460	4.734608	-1.157130
55	1	0	1.644585	3.937551	-2.599002
56	1	0	-3.905958	2.450013	1.925521
57	1	0	-3.061293	1.787738	0.488949
58	1	0	-2.753653	1.091407	2.113107
59	1	0	-3.361905	-1.552634	-0.841365
60	1	0	-4.787997	-1.386315	0.243283
61	1	0	-3.211928	-1.911443	0.907175
62	1	0	-2.269449	-2.190684	-2.115021
63	1	0	-0.929656	-3.006055	-2.995351
64	1	0	-2.627368	-3.453158	-3.345370
65	1	0	3.404970	-2.144156	-0.094191
66	1	0	3.939066	-2.562247	-1.751329
67	1	0	5.120871	-2.561251	-0.410568
68	1	0	-1.604798	3.748021	-1.884134
69	1	0	-2.694825	2.573509	-1.082265
70	1	0	-3.355649	3.760054	-2.264745

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.0080512 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 377.11304 kca/mol

Figure 2 TS2B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.914930	-0.948219	-2.726738
2	6	0	-0.726969	-2.435042	-2.746972
3	6	0	-1.630241	-3.079566	-1.698509
4	6	0	-2.997613	-2.399681	-1.806018
5	6	0	-2.805230	-0.924815	-2.015519
6	6	0	-1.613874	-0.197216	-1.738721
7	8	0	-1.456997	0.986437	-1.362445
8	1	0	-0.470931	-0.361230	-3.527821
9	17	0	1.869858	-0.459005	-1.716319
10	1	0	-0.951002	-2.817330	-3.754162
11	1	0	0.332765	-2.631060	-2.551070
12	1	0	-1.206184	-2.906277	-0.689295
13	1	0	-1.703467	-4.163811	-1.833600
14	1	0	-3.574659	-2.556847	-0.882731
15	1	0	-3.585224	-2.819466	-2.636257
16	1	0	-3.680818	-0.325061	-2.271518
17	1	0	-2.921519	0.716327	1.409957
18	8	0	-2.513205	0.053621	2.032245
19	1	0	2.180370	-2.313306	-0.735858
20	8	0	2.181208	-3.062672	-0.088206
21	1	0	-0.539184	0.391204	2.260985
22	8	0	0.369439	0.537957	2.578362
23	1	0	-2.778028	1.601406	-0.463695
24	8	0	-3.523180	1.771002	0.174768
25	1	0	0.073262	2.117495	-1.795157
26	8	0	0.470406	2.972969	-2.055878
27	1	0	5.218537	-0.410324	0.263826
28	8	0	5.525996	0.483197	0.021638
29	1	0	3.705468	-2.380766	0.820680
30	8	0	4.494307	-2.027914	1.290612
31	1	0	-3.122347	-1.705461	1.735769
32	8	0	-3.419192	-2.633055	1.628989
33	1	0	-0.294834	4.267086	-0.898216
34	8	0	-0.611181	4.896255	-0.215296
35	6	0	-2.975472	0.412096	3.318299
36	6	0	1.120359	-2.641825	0.748318
37	6	0	1.082463	0.878127	1.403966
38	6	0	-3.361334	3.123035	0.560064
39	6	0	1.815795	2.876563	-1.619655
40	6	0	4.314805	1.212797	-0.029515
41	6	0	3.943781	-1.269148	2.348782
42	6	0	-2.236931	-3.377998	1.827320
43	6	0	-0.049600	4.356398	0.963303
44	1	0	-4.065059	0.316625	3.395101
45	1	0	-2.495519	-0.295414	4.000326
46	1	0	-2.679797	1.435248	3.579717
47	1	0	1.038217	-1.541943	0.746462
48	1	0	0.155840	-3.067593	0.407544
49	1	0	1.335455	-3.008970	1.756310
50	1	0	0.900561	0.185930	0.558817
51	1	0	0.857982	1.911990	1.091541
52	1	0	2.150779	0.810273	1.676655
53	1	0	-2.432040	3.270427	1.135319
54	1	0	-3.359912	3.792245	-0.307796
55	1	0	-4.222570	3.348200	1.194901
56	1	0	2.379152	3.563962	-2.255660
57	1	0	1.881424	3.218832	-0.571750
58	1	0	2.242291	1.854570	-1.688030
59	1	0	3.697016	1.028119	0.872427
60	1	0	4.609850	2.265316	-0.054247
61	1	0	3.700069	0.979944	-0.922322
62	1	0	3.423139	-0.364172	1.971992
63	1	0	3.246488	-1.859139	2.956441
64	1	0	4.797023	-0.967449	2.961669
65	1	0	-1.493801	-3.192290	1.024567
66	1	0	-1.775419	-3.165527	2.799175
67	1	0	-2.547298	-4.425571	1.793975
68	1	0	-0.843060	3.842324	1.528389
69	1	0	0.764480	3.637512	0.750470

70	1	0	0.334058	5.191661	1.554848

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1810.9775964 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 376.53543 kca/mol
ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 231.2476ί cm-1

Figure 2 Int2B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.134487	1.916970	-1.196247
2	6	0	0.332919	0.661737	-1.940387
3	6	0	-0.862510	0.220219	-2.806439
4	6	0	-1.583908	1.521030	-3.210771
5	6	0	-1.392478	2.472179	-2.030028
6	6	0	-1.478087	1.966087	-0.653985
7	8	0	-2.163469	1.967629	0.354805
8	1	0	0.619457	2.566645	-0.743130
9	1	0	1.192595	0.942240	-2.562938
10	1	0	0.654813	-0.121096	-1.249234
11	1	0	-1.533297	-0.425110	-2.215929
12	1	0	-0.548910	-0.366003	-3.678028
13	1	0	-2.643381	1.359282	-3.448087
14	1	0	-1.115294	1.969325	-4.097497
15	1	0	-1.577040	3.535972	-2.187144
16	1	0	-3.927736	1.868179	0.152459
17	8	0	-3.956474	-1.146897	0.106176
18	8	0	-1.053259	-1.223183	0.335569
19	1	0	-2.014531	-1.200874	0.503041
20	1	0	-4.303268	-0.226599	0.023477
21	8	0	-4.840097	1.510102	0.045874
22	1	0	2.850568	3.075234	-0.039555
23	8	0	2.268053	3.769821	0.334018
24	1	0	-4.394204	-1.789251	1.936772
25	8	0	-4.533266	-1.831569	2.898813
26	1	0	-0.964647	-2.678661	-0.863963
27	8	0	-1.163393	-3.315988	-1.578860
28	17	0	2.352807	-0.291462	1.574261
29	1	0	2.319175	-1.950826	-0.069275
30	8	0	2.449930	-2.501351	-0.868314
31	1	0	3.281458	0.911341	-0.041081
32	8	0	3.713296	1.533748	-0.674138
33	1	0	4.614129	-0.528445	2.119289
34	8	0	5.581144	-0.674861	2.133474
35	6	0	-3.885528	-1.655427	-1.211755
36	6	0	-0.423976	-1.379587	1.594047
37	6	0	-5.435413	1.693852	1.316198
38	6	0	1.931217	3.219891	1.596654
39	6	0	-3.622574	-0.872925	3.396259
40	6	0	0.034700	-3.323542	-2.327797
41	6	0	3.363750	-1.723874	-1.614091
42	6	0	5.046669	1.578470	-0.205078
43	6	0	5.707415	-1.851776	1.366305
44	1	0	-4.831557	-1.531831	-1.750268
45	1	0	-3.069788	-1.166589	-1.774460
46	1	0	-3.661704	-2.719165	-1.092445
47	1	0	-0.363024	-2.445912	1.838224
48	1	0	0.620970	-0.936714	1.510911
49	1	0	-0.986099	-0.870380	2.390945
50	1	0	-4.870820	1.179803	2.112185
51	1	0	-5.526356	2.758018	1.562255
52	1	0	-6.432133	1.253047	1.231815
53	1	0	1.818743	2.122822	1.568618
54	1	0	2.695665	3.489006	2.335383
55	1	0	0.983570	3.685963	1.880022
56	1	0	-3.939230	0.147137	3.122441
57	1	0	-3.654870	-0.981663	4.483006
58	1	0	-2.590960	-1.037201	3.038552
59	1	0	0.120462	-4.326216	-2.755496
60	1	0	-0.044414	-2.594626	-3.145708
61	1	0	0.933167	-3.091608	-1.721697
62	1	0	4.275511	-1.505033	-1.032714
63	1	0	3.623505	-2.327962	-2.487332
64	1	0	2.909227	-0.778992	-1.943656
65	1	0	5.096780	1.882834	0.847838
66	1	0	5.536838	0.602852	-0.324427
67	1	0	5.553346	2.320766	-0.827583
68	1	0	5.253417	-1.738680	0.366777

69	1	0	6.782305	-2.021656	1.258535
70	1	0	5.253870	-2.713956	1.870008

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1810.99422275 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 374.47912 kca/mol

Figure 2 TS3B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.256611	-1.503693	-1.252168
2	6	0	-0.111077	-0.163718	-1.941533
3	6	0	1.175600	0.290067	-2.653615
4	6	0	1.913985	-1.010935	-3.008717
5	6	0	1.661550	-1.954583	-1.821203
6	6	0	0.913062	-1.504298	-0.000548
7	8	0	1.341294	-1.719299	1.048938
8	1	0	-0.569830	-2.234299	-1.215793
9	1	0	-0.895601	-0.412026	-2.665298
10	1	0	-0.513971	0.573338	-1.245916
11	1	0	1.785294	0.913824	-1.982247
12	1	0	0.949810	0.900746	-3.536891
13	1	0	2.984739	-0.851046	-3.179119
14	1	0	1.490558	-1.439719	-3.931673
15	1	0	1.668314	-3.024204	-2.046880
16	1	0	2.872471	-1.753757	-1.062958
17	8	0	3.909104	0.962445	0.332717
18	8	0	1.146916	1.209828	0.584150
19	1	0	2.121161	1.177047	0.727212
20	1	0	3.994444	0.028699	-0.063375
21	8	0	4.007942	-1.472267	-0.704774
22	1	0	-2.836620	-2.798258	-0.967255
23	8	0	-2.261676	-3.565197	-0.753243
24	1	0	4.558525	0.926008	2.173846
25	8	0	4.676270	0.695044	3.113635
26	1	0	1.139377	2.884580	-0.345106
27	8	0	1.339075	3.642609	-0.927606
28	17	0	-2.159194	-0.056026	1.469618
29	1	0	-2.124011	1.956518	0.238091
30	8	0	-2.241173	2.678807	-0.411341
31	1	0	-3.247871	-0.735877	-0.355744
32	8	0	-3.680186	-1.153882	-1.138559
33	1	0	-4.411572	0.108724	2.089116
34	8	0	-5.377179	0.255210	2.126879
35	6	0	4.080682	1.854779	-0.749720
36	6	0	0.522172	1.251857	1.856815
37	6	0	4.532967	-2.359114	0.250680
38	6	0	-2.221244	-3.512105	0.662915
39	6	0	3.669401	-0.274797	3.314056
40	6	0	0.176707	3.717424	-1.727513
41	6	0	-3.198087	2.136062	-1.297460
42	6	0	-5.017375	-1.330876	-0.711358
43	6	0	-5.489392	1.589690	1.682994
44	1	0	5.067515	1.740872	-1.211554
45	1	0	3.294213	1.695785	-1.508111
46	1	0	3.983916	2.857044	-0.323683
47	1	0	0.433404	2.292571	2.183540
48	1	0	-0.504991	0.790905	1.719454
49	1	0	1.099805	0.691660	2.608339
50	1	0	4.149062	-2.126633	1.259460
51	1	0	4.292947	-3.401652	0.011009
52	1	0	5.619656	-2.230904	0.246364
53	1	0	-2.048319	-2.489720	1.039818
54	1	0	-3.154716	-3.901669	1.087246
55	1	0	-1.396615	-4.166503	0.957489
56	1	0	3.812986	-1.148753	2.655136
57	1	0	3.766436	-0.584653	4.357319
58	1	0	2.659546	0.139799	3.147054
59	1	0	0.104008	4.756697	-2.058511
60	1	0	0.292714	3.069619	-2.607404
61	1	0	-0.743862	3.426387	-1.183280
62	1	0	-4.103479	1.803161	-0.762157
63	1	0	-3.456581	2.945852	-1.984607
64	1	0	-2.781195	1.292763	-1.865381
65	1	0	-5.073199	-1.960530	0.185736
66	1	0	-5.497514	-0.364148	-0.510213
67	1	0	-5.525774	-1.827646	-1.541884

68	1	0	-5.032595	1.728578	0.687945
69	1	0	-6.562388	1.790563	1.619872
70	1	0	-5.030363	2.291751	2.389366

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1810.94124663 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 370.86482 kca/mol
ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 1160.3737i cm-1

Figure 2 product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.787908	-0.786799	-1.694088
2	6	0	0.386393	0.603015	-2.237505
3	6	0	1.714153	1.277250	-2.615651
4	6	0	2.525950	0.123608	-3.231097
5	6	0	2.158952	-1.121322	-2.385046
6	6	0	0.903359	-0.949298	-0.188116
7	8	0	1.123756	-2.008184	0.346890
8	1	0	0.027865	-1.535095	-1.953085
9	1	0	-0.209286	0.447914	-3.147336
10	1	0	-0.233426	1.180180	-1.546349
11	1	0	2.210996	1.672893	-1.713889
12	1	0	1.580700	2.124925	-3.299726
13	1	0	3.606123	0.305352	-3.231137
14	1	0	2.216408	-0.020960	-4.275174
15	1	0	2.076766	-2.023877	-2.998290
16	1	0	2.939777	-1.313710	-1.643437
17	8	0	3.548655	0.968752	0.904398
18	8	0	0.753496	0.244748	0.529551
19	1	0	2.581712	0.853596	0.812609
20	1	0	4.692161	-0.183866	-0.151263
21	8	0	5.246931	-0.780265	-0.687730
22	1	0	-2.793315	-2.255547	-1.766403
23	8	0	-2.078037	-2.916503	-1.862511
24	1	0	4.050304	0.201095	2.701197
25	8	0	4.195514	-0.364985	3.478338
26	1	0	0.462312	2.523364	0.367951
27	8	0	0.938584	3.358249	0.257042
28	17	0	-2.626769	-0.433391	1.600156
29	1	0	-2.275832	1.609501	0.536186
30	8	0	-2.237827	2.408123	-0.031268
31	1	0	-3.715419	-0.801841	-0.343397
32	8	0	-4.147063	-1.024196	-1.200733
33	1	0	-4.905864	-0.157473	2.126163
34	8	0	-5.858044	0.054643	2.086646
35	6	0	3.793159	2.272267	0.407806
36	6	0	0.253132	0.093695	1.877810
37	6	0	5.414301	-1.900960	0.154826
38	6	0	-1.849157	-3.289477	-0.515187
39	6	0	3.402589	-1.500021	3.194275
40	6	0	0.068946	4.032332	-0.633032
41	6	0	-3.092182	2.051701	-1.100058
42	6	0	-5.239834	-1.830420	-0.805722
43	6	0	-5.846170	1.277485	1.382956
44	1	0	4.880819	2.349717	0.331371
45	1	0	3.333916	2.403644	-0.585954
46	1	0	3.413249	3.033823	1.097878
47	1	0	0.369234	1.105583	2.272791
48	1	0	-0.854649	-0.202843	1.849812
49	1	0	0.860366	-0.607016	2.467136
50	1	0	4.502130	-2.144813	0.723843
51	1	0	5.669998	-2.733455	-0.505726
52	1	0	6.237283	-1.730823	0.859752
53	1	0	-1.842562	-2.422617	0.166495
54	1	0	-2.614027	-4.003513	-0.183925
55	1	0	-0.871324	-3.778320	-0.507642
56	1	0	3.748985	-2.012700	2.280980
57	1	0	3.528645	-2.161776	4.054283
58	1	0	2.336703	-1.240436	3.080303
59	1	0	0.120534	5.094241	-0.381104
60	1	0	0.420574	3.885812	-1.662485
61	1	0	-0.966045	3.655405	-0.533036
62	1	0	-4.076006	1.714740	-0.733384
63	1	0	-3.213505	2.959586	-1.697156
64	1	0	-2.644378	1.263481	-1.719823
65	1	0	-4.899643	-2.746314	-0.305125
66	1	0	-5.922942	-1.282242	-0.144891

67	1	0	-5.757471	-2.093554	-1.732177
68	1	0	-5.192308	1.239868	0.494604
69	1	0	-6.878894	1.451978	1.068428
70	1	0	-5.522297	2.102344	2.029449

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.05311283 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 375.80902 kca/mol

Figure 4 Int2B’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.924499	0.308869	-0.164466
2	6	0	-0.570634	0.082182	-1.637780
3	6	0	-0.051744	1.440426	-2.160743
4	6	0	0.549085	2.189466	-0.946530
5	6	0	-0.221970	1.666898	0.265718
6	6	0	-1.671118	1.517845	0.153474
7	8	0	-2.761844	2.045515	0.308497
8	1	0	-0.988439	-0.553233	0.506369
9	1	0	0.218059	-0.688773	-1.689335
10	1	0	-1.432346	-0.299615	-2.196619
11	1	0	-0.886909	2.031356	-2.573927
12	1	0	0.686998	1.303925	-2.965745
13	1	0	0.444317	3.275138	-1.048845
14	1	0	1.614361	1.965747	-0.802734
15	1	0	0.205913	1.791289	1.264225
16	17	0	-1.429536	-0.588134	3.334205
17	1	0	2.386366	-0.367525	1.650052
18	8	0	3.051452	-0.476061	0.908757
19	1	0	3.003166	-0.930941	-0.927701
20	8	0	3.251901	-1.230951	-1.827434
21	1	0	3.711314	1.298591	0.862053
22	8	0	3.906514	2.256772	0.823867
23	1	0	-3.909994	-1.200208	-1.277360
24	8	0	-3.562939	-1.694997	-2.050387
25	1	0	-2.422549	3.938101	-0.317004
26	8	0	-2.093652	4.678480	-0.856032
27	1	0	-1.323473	-2.532158	2.159573
28	8	0	-1.086685	-3.213985	1.495621
29	1	0	-4.048806	0.605005	0.287580
30	8	0	-4.553813	-0.224092	0.193155
31	1	0	2.335303	-2.667371	-2.700489
32	8	0	1.797476	-3.330373	-3.173205
33	1	0	0.605043	-0.300606	3.212369
34	8	0	1.580712	-0.089277	3.130463
35	6	0	4.018834	-1.355351	1.452713
36	6	0	3.157313	-0.090217	-2.652512
37	6	0	4.727560	2.393339	-0.312120
38	6	0	-2.852923	-2.761887	-1.456007
39	6	0	-2.465600	4.316839	-2.167854
40	6	0	0.221700	-2.815815	1.153746
41	6	0	-4.250573	-0.936988	1.383871
42	6	0	0.590512	-3.330356	-2.442149
43	6	0	1.651279	1.284174	3.455606
44	1	0	4.459828	-0.946346	2.369315
45	1	0	3.578665	-2.337619	1.663243
46	1	0	4.793295	-1.454172	0.686450
47	1	0	3.772241	0.741322	-2.272101
48	1	0	3.536723	-0.414599	-3.624786
49	1	0	2.115883	0.260467	-2.761332
50	1	0	5.689080	1.880940	-0.183629
51	1	0	4.237132	2.010529	-1.222613
52	1	0	4.900468	3.467441	-0.416868
53	1	0	-3.499799	-3.378504	-0.819944
54	1	0	-2.477592	-3.363034	-2.290125
55	1	0	-1.999465	-2.399698	-0.862637
56	1	0	-3.548088	4.173114	-2.266311
57	1	0	-2.151775	5.154048	-2.796729
58	1	0	-1.944847	3.400798	-2.496456
59	1	0	0.260334	-1.733007	0.942236
60	1	0	0.942312	-3.053382	1.946295
61	1	0	0.482570	-3.373316	0.242561
62	1	0	-3.204590	-0.816538	1.717132
63	1	0	-4.925633	-0.617930	2.185598
64	1	0	-4.444133	-1.987444	1.144521
65	1	0	0.165824	-2.315531	-2.343948

66	1	0	-0.100927	-3.959974	-3.008443
67	1	0	0.722051	-3.748329	-1.429588
68	1	0	1.072496	1.890514	2.740179
69	1	0	1.285514	1.472243	4.470810
70	1	0	2.709902	1.552776	3.387002

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.01179683 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 375.66179 kca/mol

Figure 4 TS4B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230094	-0.282564	0.073171
2	6	0	0.124795	-0.692117	-1.363785
3	6	0	0.847723	0.517276	-2.023801
4	6	0	1.030438	1.617678	-0.935741
5	6	0	0.653655	0.945847	0.373169
6	6	0	-1.282778	0.699954	0.146137
7	8	0	-1.908747	1.385897	-0.658847
8	1	0	-0.243330	-1.106912	0.794487
9	1	0	0.796130	-1.560526	-1.281122
10	1	0	-0.762509	-1.024533	-1.913486
11	1	0	0.273919	0.902372	-2.873882
12	1	0	1.823426	0.187495	-2.418281
13	1	0	0.389393	2.484092	-1.168951
14	1	0	2.062729	1.990857	-0.905550
15	1	0	0.576454	1.509738	1.298070
16	17	0	-2.052210	0.740814	2.030835
17	1	0	2.134178	0.252491	0.810045
18	8	0	3.120848	-0.068239	1.001938
19	1	0	3.588476	-1.465717	0.012209
20	8	0	3.802792	-2.239046	-0.565878
21	1	0	4.226382	1.369850	0.473386
22	8	0	4.752170	2.068544	0.033349
23	1	0	-3.435076	-1.673873	-1.977939
24	8	0	-2.989493	-2.491597	-2.284090
25	1	0	-1.828287	3.266006	-1.125806
26	8	0	-1.741934	4.154657	-1.517729
27	1	0	-2.508940	-1.702632	2.287780
28	8	0	-2.557991	-2.671514	2.252850
29	1	0	-3.483844	0.522066	-1.166008
30	8	0	-4.232216	-0.081197	-1.353467
31	1	0	2.380821	-3.337814	0.013236
32	8	0	1.619041	-3.773875	0.446496
33	1	0	-0.873674	2.786003	2.770301
34	8	0	-0.264603	3.523293	2.932382
35	6	0	3.166420	-0.405616	2.372343
36	6	0	3.828849	-1.685440	-1.864747
37	6	0	5.675473	1.339970	-0.741896
38	6	0	-2.717791	-3.180087	-1.082058
39	6	0	-1.606631	3.875063	-2.893382
40	6	0	-1.209169	-3.064124	2.403667
41	6	0	-4.752730	-0.353109	-0.065189
42	6	0	0.794943	-4.153569	-0.631642
43	6	0	-0.399775	4.307832	1.764468
44	1	0	2.878863	0.445153	3.000827
45	1	0	2.510832	-1.257447	2.589457
46	1	0	4.204349	-0.680333	2.581312
47	1	0	4.650262	-0.956794	-1.964419
48	1	0	3.999372	-2.526652	-2.540658
49	1	0	2.881528	-1.181656	-2.125663
50	1	0	6.427455	0.847681	-0.112156
51	1	0	5.189025	0.577373	-1.373618
52	1	0	6.169469	2.077294	-1.380332
53	1	0	-3.613823	-3.293119	-0.458600
54	1	0	-2.355457	-4.166995	-1.384850
55	1	0	-1.931884	-2.676649	-0.497460
56	1	0	-2.533717	3.466416	-3.314324
57	1	0	-1.389593	4.836496	-3.366848
58	1	0	-0.782951	3.175897	-3.093249
59	1	0	-0.544410	-2.531980	1.702300
60	1	0	-0.859606	-2.903074	3.430104
61	1	0	-1.191731	-4.133514	2.174872
62	1	0	-3.964109	-0.416386	0.699238
63	1	0	-5.473504	0.421500	0.219759
64	1	0	-5.266238	-1.315919	-0.147790
65	1	0	0.557883	-3.293340	-1.280224

66	1	0	1.250648	-4.950617	-1.230739
67	1	0	-0.129710	-4.520340	-0.172649
68	1	0	-0.186350	3.732266	0.852232
69	1	0	-1.402092	4.747107	1.689413
70	1	0	0.337898	5.107475	1.871090

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1810.96514879 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 372.31995 kca/mol
ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 521.8904í cm-1

Figure 4 Int3B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.853143	-1.002969	0.014527
2	6	0	0.277933	0.230988	-0.712565
3	6	0	-0.328417	-0.380527	-1.985786
4	6	0	0.714352	-1.422131	-2.423827
5	6	0	1.291703	-2.009833	-1.110689
6	6	0	1.933548	-0.662219	0.978848
7	8	0	2.397041	0.383146	1.308424
8	1	0	0.047587	-1.470675	0.608348
9	1	0	-0.459082	0.758275	-0.089434
10	1	0	1.069077	0.940512	-0.987924
11	1	0	-0.518715	0.389499	-2.753496
12	1	0	-1.284489	-0.876433	-1.750594
13	1	0	1.511402	-0.926433	-2.994251
14	1	0	0.284196	-2.205646	-3.055090
15	1	0	2.384373	-2.117450	-1.171543
16	17	0	2.669551	-2.193379	1.797178
17	1	0	0.866718	-2.991948	-0.900697
18	8	0	-1.980015	-1.791252	1.213435
19	1	0	-3.361755	-1.161614	0.545528
20	8	0	-4.151388	-0.761178	0.048519
21	1	0	-1.713369	-2.947046	-0.085142
22	8	0	-1.526156	-3.542559	-0.866671
23	1	0	1.378782	4.056047	0.560349
24	8	0	1.000982	4.503560	-0.231786
25	1	0	1.445366	3.565990	-1.812189
26	8	0	1.692371	3.104914	-2.641495
27	1	0	-1.413825	-0.324646	2.028055
28	8	0	-1.082528	0.505556	2.466470
29	1	0	2.029141	2.214455	1.769288
30	8	0	1.991100	3.152957	2.023698
31	1	0	-4.005172	1.073748	-0.241183
32	8	0	-3.904059	2.022743	-0.485536
33	1	0	4.662810	-2.665777	0.112466
34	8	0	5.241566	-2.760355	-0.658017
35	6	0	-2.305075	-2.592677	2.296671
36	6	0	-4.010272	-1.289943	-1.250183
37	6	0	-2.573326	-4.480615	-0.853057
38	6	0	-0.394850	4.358846	-0.062102
39	6	0	0.465007	2.936134	-3.315110
40	6	0	-2.187809	1.370084	2.334440
41	6	0	0.978991	3.187893	3.014287
42	6	0	-2.778265	2.005408	-1.332094
43	6	0	4.994306	-1.578370	-1.389702
44	1	0	-1.395169	-2.959472	2.792679
45	1	0	-2.899388	-2.039024	3.039483
46	1	0	-2.896168	-3.468861	1.984237
47	1	0	-4.165283	-2.381381	-1.257224
48	1	0	-4.776683	-0.810628	-1.866409
49	1	0	-3.012052	-1.071676	-1.671085
50	1	0	-2.624432	-5.031512	0.094997
51	1	0	-3.545633	-3.992814	-1.036126
52	1	0	-2.363497	-5.181124	-1.666350
53	1	0	-0.756459	4.962339	0.778927
54	1	0	-0.840165	4.722888	-0.993743
55	1	0	-0.685077	3.308377	0.094876
56	1	0	-0.161938	3.835936	-3.279289
57	1	0	0.729327	2.716337	-4.352847
58	1	0	-0.102253	2.083946	-2.899606
59	1	0	-3.128254	0.824874	2.191215
60	1	0	-2.243944	1.968229	3.249888
61	1	0	-2.025585	2.043356	1.480082
62	1	0	1.198702	2.504144	3.841676
63	1	0	0.979037	4.218130	3.380902

64	1	0	-0.006241	2.947666	2.588798
65	1	0	-1.888849	1.574546	-0.832271
66	1	0	-2.968138	1.438369	-2.253977
67	1	0	-2.575531	3.050991	-1.586026
68	1	0	3.926104	-1.479120	-1.644615
69	1	0	5.324699	-0.686074	-0.844813
70	1	0	5.580331	-1.682514	-2.306155

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.02253829 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 375.98648 kca/mol

Figure 4 TS5B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739846	-0.899535	-2.062368
2	6	0	-0.511236	-0.068382	-2.474472
3	6	0	-0.027830	0.978795	-3.502059
4	6	0	1.473311	1.132834	-3.208690
5	6	0	1.920913	-0.306474	-2.908950
6	6	0	1.105249	-0.681446	-0.621622
7	8	0	1.128007	0.336767	-0.003807
8	1	0	0.602243	-1.965807	-2.231313
9	1	0	-1.280375	-0.741795	-2.862505
10	1	0	-0.944142	0.430333	-1.608914
11	1	0	-0.593773	1.910331	-3.405053
12	1	0	-0.161736	0.609379	-4.528691
13	1	0	1.625459	1.764304	-2.313197
14	1	0	2.040403	1.585507	-4.031133
15	1	0	2.895911	-0.366999	-2.412731
16	17	0	2.082935	-2.143936	0.091827
17	1	0	1.988581	-0.883939	-3.839400
18	8	0	-1.144456	-1.544019	0.182720
19	1	0	-2.099513	-0.782046	0.054283
20	8	0	-3.038388	0.016068	-0.118409
21	1	0	-1.399123	-2.847477	-0.974377
22	8	0	-1.516531	-3.465941	-1.741083
23	1	0	-2.813566	1.616156	-0.967126
24	8	0	-2.701723	2.468565	-1.457770
25	1	0	1.745973	3.063930	1.475080
26	8	0	2.123112	3.758772	0.903303
27	1	0	4.220941	-0.733065	-0.262081
28	8	0	4.906996	-0.162896	-0.639600
29	1	0	1.283552	0.922694	1.769271
30	8	0	1.244532	1.485437	2.562405
31	1	0	-3.788680	0.393619	1.480544
32	8	0	-4.153160	0.642639	2.366520
33	1	0	1.112895	-3.024527	2.661229
34	8	0	1.620516	-3.076377	3.488983
35	6	0	-1.056063	-2.042331	1.487635
36	6	0	-4.047809	-0.542041	-0.915259
37	6	0	-2.855800	-3.883048	-1.621058
38	6	0	-2.382597	3.387445	-0.441028
39	6	0	1.374679	3.667709	-0.289962
40	6	0	4.505389	1.136227	-0.251052
41	6	0	-0.087982	1.310104	3.009107
42	6	0	-3.642728	1.939690	2.558047
43	6	0	2.261392	-1.817850	3.527447
44	1	0	-0.174167	-2.701299	1.538507
45	1	0	-0.920261	-1.224195	2.217505
46	1	0	-1.948225	-2.617656	1.762363
47	1	0	-3.777342	-0.469827	-1.978221
48	1	0	-4.218520	-1.606724	-0.681908
49	1	0	-4.974855	0.015851	-0.742825
50	1	0	-2.961499	-4.643001	-0.836352
51	1	0	-3.537004	-3.043666	-1.399277
52	1	0	-3.123337	-4.327100	-2.583982
53	1	0	-3.102024	3.351087	0.394225
54	1	0	-1.368862	3.213100	-0.042561
55	1	0	-2.416383	4.375930	-0.907311
56	1	0	0.289519	3.612604	-0.105090
57	1	0	1.603893	4.583043	-0.842175
58	1	0	1.676801	2.796686	-0.899296
59	1	0	3.574703	1.435808	-0.754515
60	1	0	4.374999	1.222521	0.834387
61	1	0	5.318534	1.791367	-0.573879
62	1	0	-0.403161	0.252914	2.962234
63	1	0	-0.094251	1.653431	4.046661

64	1	0	-0.798772	1.915637	2.421383
65	1	0	-2.541133	1.938262	2.641504
66	1	0	-3.922372	2.625346	1.740406
67	1	0	-4.074844	2.299028	3.495707
68	1	0	2.827847	-1.623223	2.606231
69	1	0	1.537135	-1.006068	3.682467
70	1	0	2.945018	-1.865854	4.378464

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.01031344 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 373.34942 kca/mol
ONIOM(rb3lyp / 6-31g* : PM3) Frequency : 878.8593í cm-1

Figure 4 product’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.294297	-1.136955	1.655297
2	6	0	1.189664	-1.187890	2.182627
3	6	0	1.125058	-0.705638	3.651154
4	6	0	-0.143695	0.160281	3.710151
5	6	0	-1.134590	-0.637982	2.852461
6	6	0	-0.402997	-0.208104	0.465420
7	8	0	-0.845658	0.917674	0.475198
8	1	0	-0.624017	-2.119261	1.302016
9	1	0	1.612557	-2.193628	2.092187
10	1	0	1.849009	-0.528749	1.605426
11	1	0	2.036463	-0.175012	3.949432
12	1	0	1.012506	-1.565624	4.324444
13	1	0	0.047146	1.143748	3.244671
14	1	0	-0.498648	0.338238	4.731751
15	1	0	-2.024180	-0.079678	2.535471
16	17	0	-3.399427	-1.210202	-1.267584
17	1	0	-1.485919	-1.511616	3.415202
18	8	0	0.129903	-0.816597	-0.662306
19	1	0	1.770164	-1.609547	-0.779276
20	8	0	2.667963	-1.950205	-0.976207
21	1	0	-2.451757	-3.064899	-0.219539
22	8	0	-1.821579	-3.798816	-0.070237
23	1	0	3.959562	-1.327523	0.339854
24	8	0	4.588358	-0.983903	1.001322
25	1	0	1.143536	3.733603	0.659977
26	8	0	1.834431	3.929682	1.326156
27	1	0	-4.374055	-0.523844	0.726517
28	8	0	-4.752944	-0.180895	1.562121
29	1	0	-0.625353	2.608980	-0.552220
30	8	0	-0.141523	3.441646	-0.702590
31	1	0	3.021291	-0.885326	-2.627693
32	8	0	3.104839	-0.249935	-3.359648
33	1	0	-2.749808	0.849649	-2.187737
34	8	0	-2.537274	1.755721	-2.505709
35	6	0	-0.263450	-0.286904	-1.941449
36	6	0	2.537578	-3.354429	-0.845020
37	6	0	-1.228406	-3.834034	-1.353538
38	6	0	4.646645	0.395856	0.713440
39	6	0	1.947510	2.735355	2.064341
40	6	0	-4.212989	1.118427	1.632127
41	6	0	0.544648	3.186793	-1.912656
42	6	0	3.423617	0.966396	-2.719211
43	6	0	-3.466337	2.559230	-1.813944
44	1	0	-1.361924	-0.368575	-2.060041
45	1	0	0.070966	0.752179	-2.080553
46	1	0	0.256699	-0.952607	-2.634635
47	1	0	2.598523	-3.635040	0.213763
48	1	0	1.587105	-3.720942	-1.265794
49	1	0	3.382807	-3.779796	-1.390922
50	1	0	-1.545073	-2.965028	-1.946388
51	1	0	-0.134418	-3.825210	-1.226167
52	1	0	-1.516939	-4.762546	-1.857453
53	1	0	4.826365	0.593765	-0.355997
54	1	0	3.718351	0.908882	1.019460
55	1	0	5.482809	0.780577	1.302278
56	1	0	2.419782	1.933623	1.470155
57	1	0	2.598768	2.978457	2.908478
58	1	0	0.979817	2.368321	2.446935
59	1	0	-3.182432	1.083686	2.021620
60	1	0	-4.209180	1.631431	0.657762
61	1	0	-4.842736	1.671795	2.334322

62	1	0	0.006067	2.464291	-2.545207
63	1	0	0.636240	4.147729	-2.423797
64	1	0	1.551364	2.781886	-1.707331
65	1	0	2.528569	1.435325	-2.271678
66	1	0	4.191506	0.845086	-1.937708
67	1	0	3.807575	1.616418	-3.509650
68	1	0	-4.470592	2.459408	-2.243326
69	1	0	-3.509416	2.315061	-0.740348
70	1	0	-3.118722	3.588364	-1.941326

ONIOM(rb3lyp / 6-31g* : PM3)//b3lyp / 6-311+G(d,p) SCF Done : -1811.06423201 a.u.
ONIOM(rb3lyp / 6-31g* : PM3) Zero-point vibrational energy : 377.50103 kca/mol