Supporting information

Complete Reversal in Regioselectivity in the Baeyer-Villiger Reaction of an α-CF_3-Ketone and Theoretical Rationale for Axial Orientation of Sterically Demanding CF_3 Group at the Transition State

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General:

^{1}H NMR and ^{13}C NMR were measured on Varian Gemini 300 (300 MHz) spectrometers and ^{19}F NMR was measured on Varian Gemini 400 (400 MHz) spectrometers. Chemical shift of ^{1}H NMR was expressed in parts per million downfield from tetramethylsilane as an internal standard (δ=0) in $CDCl_3$. Chemical shifts of ^{13}C NMR were expressed in parts per million downfield from $CDCl_3$ as an internal standard (δ = 77.0) in $CDCl_3$. Chemical shifts of ^{19}F NMR were expressed in parts per million downfield from BTF as an internal standard (δ=-63.24) in $CDCl_3$. Analytical thin layer chromatography (TLC) were performed on a glass plates and /or aluminum sheets pre-coated with silica gel (Merck Kieselgal 60 F_{254}, layer thickness 0.25 and 0.2 mm). Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$ and phosphomolybdic acid. Column chromatography was performed on Merck Kieselgel 60 and KANTO Silica Gel 60N (spherical, neutral), employing hexane ethyl acetate mixture as an eluent unless otherwise noted. All experiments were carried out under argon atmosphere unless otherwise noted. The calculations were performed with a GAUSSIAN 98 program package using the Hartree-Fock method.

Preparation of trifluoroperacetic acid (TFPA)

To a solution of trifluoroacetic anhydride (TFAA)(0.48 ml, 3.4 mmol) in dichloromethane (4 ml) was added 60% hydrogen peroxide (85 mg, 1.4 mmol) at 0 ºC and stirred for 1 h at room temperature. The resultant solution was directly used as 0.33 mol/l TFPA solution of dichloromethane containing TFA (TFPA : TFA=2 : 7).

General procedure for Baeyer-Villiger reaction

a) TFPA

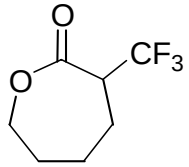
To the TFPA (0.6 ml) was added dichloromethane (0.4 ml) at room temperature. And then 2-trifluoromethyl-cyclohexanone (16.6 mg, 0.1 mmol) was added to the mixture at the temperature. After stirring for 16 h at the temperature (NMR yield at this stage was

quantitative), the reaction mixture was directly transferred to silica gel column chromatography (dichloromethane only). Purification by column chromatography gave 2-trifluoromethyl-6-hexanolide in 89% yield.

b) *m*CPBA

To a solution of *m*CPBA (80% purity) (43.1 mg, 0.2 mmol) and an additive (if needed) in dichloromethane was added 2-trifluoromethyl cyclohexanone (16.6 mg, 0.1 mmol) at room temperature under argon atmosphere. The reaction was monitored by ^{19}F-NMR using BTF as an internal standard.

2-Trifluoromethyl-6-hexanolide



^{1}H NMR ($CDCl_3$, 300 MHz)

δ 1.55~1.90 (m, 3H), 1.95~2.28 (m, 3H), 3.24~3.40 (m, 1H), 4.19 (dd, *J*=10.7, 13.1 Hz, 1H), 4.39 (dm, *J*=13.2 Hz, 1H)

^{13}C NMR ($CDCl_3$, 75 MHz)

δ 23.8, 27.2, 28.3, 47.7(q, *J*=27.3 Hz), 69.0, 124.5(q, *J*=278.3 Hz), 168.5

^{19}F NMR ($CDCl_3$, 376 Hz)

δ -70.5 (d, *J*=6.8 Hz)

***Ab initio* calculations on CP1~CP8, TS1~TS8**

CP1

E(MP2/6-31G**//HF/6-31G*) = -1245.5877251139 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.755948	0.469687	0.638352
2	1	0	1.205119	2.096903	1.903721
3	6	0	1.284968	2.843127	-0.120264
4	6	0	2.732916	2.443889	-0.402236
5	6	0	2.834088	0.965774	-0.778557
6	6	0	2.207823	0.060754	0.298364
7	8	0	0.031718	0.150938	-0.549722
8	6	0	2.399834	-1.399933	-0.080629
9	1	0	2.332302	0.794616	-1.723733
10	1	0	2.753318	0.181209	1.228466
11	1	0	3.872214	0.683840	-0.911395
12	1	0	3.142223	3.047246	-1.206114
13	1	0	0.698077	2.763100	-1.030539
14	1	0	3.342669	2.639469	0.477913

15	1	0	1.234464	3.879999	0.196309
16	8	0	-1.293781	0.511005	-0.404750
17	6	0	0.677731	1.957344	0.965423
18	6	0	-2.074145	-0.535603	-0.162387
19	1	0	-0.358738	2.207247	1.148747
20	8	0	0.224810	-0.198273	1.711679
21	1	0	0.239268	-1.137210	1.565605
22	8	0	-1.756150	-1.651122	0.004410
23	6	0	-3.529769	-0.054752	-0.145694
24	9	0	-3.868449	0.392642	-1.336072
25	9	0	-4.324269	-1.039130	0.179015
26	9	0	-3.680759	0.920219	0.725224
27	9	0	1.785579	-2.229581	0.760294
28	9	0	3.688801	-1.705954	-0.037910
29	9	0	1.971313	-1.689143	-1.292345

CP2

E(MP2/6-31G**//HF/6-31G*) = -1245.5823330687 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.129563	-0.810452	0.573718
2	1	0	-2.751835	-1.781072	1.515126
3	6	0	-3.079045	-1.996683	-0.607024
4	6	0	-3.760735	-0.647888	-0.830238
5	6	0	-2.730843	0.476878	-0.927891
6	6	0	-1.826796	0.538848	0.316903
7	8	0	-0.269852	-1.220899	-0.488952
8	6	0	-0.966155	1.797359	0.251992
9	1	0	-2.113042	0.331616	-1.806718
10	1	0	-2.444069	0.690585	1.195805
11	1	0	-3.231332	1.430773	-1.044993
12	1	0	-4.355615	-0.673095	-1.737566
13	1	0	-2.501408	-2.266918	-1.485293
14	1	0	-4.447497	-0.444793	-0.010618
15	1	0	-3.818643	-2.777721	-0.462350
16	8	0	0.839655	-0.403200	-0.572531
17	6	0	-2.164533	-1.940482	0.616271
18	6	0	1.906565	-0.947562	-0.005247
19	1	0	-1.626763	-2.875204	0.742434
20	8	0	-0.429039	-0.731988	1.750143
21	1	0	-0.030418	-1.574449	1.941665
22	8	0	1.968030	-1.953188	0.597557
23	6	0	3.117512	-0.048111	-0.281185
24	9	0	2.879833	1.182512	0.107953
25	9	0	4.163464	-0.502382	0.357861
26	9	0	3.377546	-0.040408	-1.571500
27	9	0	-0.012703	1.849949	1.158153
28	9	0	-1.753431	2.850869	0.459105

29	9	0	-0.404505	1.979797	-0.931687

CP3

E(MP2/6-31G**//HF/6-31G*) = -1245.5856350179 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.620751	0.046141	0.181152
2	1	0	1.407624	0.918404	1.936597
3	6	0	1.246202	2.494181	0.469028
4	6	0	2.567366	2.245866	-0.259695
5	6	0	2.425645	1.111076	-1.277320
6	6	0	1.891080	-0.202916	-0.669670
7	8	0	-0.325054	0.319208	-0.862879
8	1	0	1.604899	-0.861378	-1.483993
9	1	0	1.725982	1.414430	-2.047786
10	6	0	2.959938	-0.987734	0.076514
11	1	0	3.368330	0.916941	-1.772160
12	1	0	2.881976	3.145606	-0.779181
13	1	0	0.503949	2.857903	-0.235760
14	1	0	3.346534	2.012050	0.459365
15	1	0	1.370297	3.267381	1.220361
16	8	0	-1.569115	0.570187	-0.319859
17	6	0	0.735931	1.221221	1.144185
18	6	0	-2.383717	-0.469840	-0.444187
19	1	0	-0.234632	1.378567	1.595981
20	8	0	0.203746	-1.037656	0.907531
21	1	0	0.131661	-1.809826	0.357042
22	8	0	-2.140242	-1.529277	-0.884128
23	6	0	-3.767341	-0.063851	0.076523
24	9	0	-4.269427	0.886773	-0.682696
25	9	0	-4.573160	-1.091531	0.057375
26	9	0	-3.680097	0.387594	1.308905
27	9	0	3.305699	-0.453286	1.236885
28	9	0	4.062861	-1.073422	-0.653149
29	9	0	2.572297	-2.232196	0.315461

CP4

E(MP2/6-31G**//HF/6-31G*) = -1245.5854405196 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.733157	-0.577387	-0.544695
2	1	0	2.422253	-1.207531	-1.649913
3	6	0	2.365992	-2.427524	0.133569
4	6	0	3.030638	-1.459105	1.113552
5	6	0	2.029128	-0.417858	1.621418

6	6	0	1.343998	0.381879	0.495299
7	8	0	-0.313669	-1.328078	0.083044
8	1	0	0.530557	0.954688	0.921235
9	1	0	1.246996	-0.922407	2.178025
10	6	0	2.255436	1.441666	-0.112291
11	1	0	2.505517	0.268571	2.308447
12	1	0	3.429688	-2.008681	1.960318
13	1	0	1.633571	-3.031469	0.659872
14	1	0	3.872717	-0.968571	0.635678
15	1	0	3.100743	-3.111815	-0.278313
16	8	0	-1.325621	-0.487528	0.508110
17	6	0	1.684061	-1.679262	-1.015308
18	6	0	-2.370530	-0.512406	-0.309645
19	1	0	1.112902	-2.366296	-1.633118
20	8	0	0.215406	0.154393	-1.580359
21	1	0	-0.161277	-0.428556	-2.231013
22	8	0	-2.476466	-1.084481	-1.327891
23	6	0	-3.487629	0.337185	0.307339
24	9	0	-3.048306	1.545456	0.583983
25	9	0	-4.491270	0.430056	-0.523101
26	9	0	-3.906526	-0.221389	1.423138
27	9	0	3.189428	0.943636	-0.914682
28	9	0	2.893240	2.100191	0.848080
29	9	0	1.586062	2.342546	-0.802962

CP5

E(MP2/6-31G**//HF/6-31G*) = -1245.586794135 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.743771	0.573752	-0.096463
2	1	0	2.299638	0.050117	-1.467704
3	6	0	3.218049	0.751904	0.352849
4	6	0	3.184288	2.236049	-0.015555
5	6	0	1.804664	2.844029	0.231502
6	6	0	0.716283	2.047458	-0.488710
7	8	0	0.374455	0.489803	1.223525
8	1	0	-0.263314	2.441009	-0.253179
9	1	0	1.593677	2.858113	1.295624
10	1	0	0.847877	2.111369	-1.564537
11	1	0	1.779944	3.873370	-0.111758
12	1	0	3.938027	2.765106	0.558784
13	1	0	3.068197	0.633577	1.420731
14	1	0	3.452138	2.352130	-1.064234
15	1	0	4.187783	0.334905	0.114974
16	1	0	0.378188	-0.413520	1.520065
17	6	0	2.132027	-0.039976	-0.399805
18	6	0	2.249853	-1.528807	-0.105643
19	8	0	-0.150324	-0.181726	-0.909004

20	8	0	-1.438727	0.292697	-0.752336
21	6	0	-2.168322	-0.490218	0.032717
22	8	0	-1.823758	-1.436531	0.632466
23	6	0	-3.607114	0.039167	0.034805
24	9	0	-4.338733	-0.651850	0.867510
25	9	0	-4.124252	-0.059356	-1.171120
26	9	0	-3.629514	1.304358	0.396832
27	9	0	1.912946	-1.821053	1.150146
28	9	0	3.499349	-1.936359	-0.269976
29	9	0	1.500614	-2.271327	-0.893410

CP6

E(MP2/6-31G**//HF/6-31G*) = -1245.5806957932 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.059128	-0.807734	0.206738
2	1	0	-2.183230	0.573017	1.360800
3	6	0	-3.122611	0.398766	-0.567113
4	6	0	-3.986648	-0.801738	-0.175761
5	6	0	-3.190463	-2.105321	-0.198618
6	6	0	-1.923638	-1.991523	0.650765
7	8	0	-0.611497	-0.947608	-1.081552
8	1	0	-1.319281	-2.890006	0.574930
9	1	0	-2.919068	-2.348558	-1.221184
10	1	0	-2.177376	-1.868793	1.698759
11	1	0	-3.795796	-2.926471	0.171517
12	1	0	-4.835876	-0.870580	-0.847990
13	1	0	-2.815660	0.319331	-1.603938
14	1	0	-4.390864	-0.641444	0.822135
15	1	0	-3.700949	1.307190	-0.469139
16	1	0	-0.188386	-1.793813	-1.183369
17	6	0	-1.869152	0.499395	0.324824
18	6	0	-1.118420	1.798971	0.067175
19	8	0	0.033077	-0.885391	1.128942
20	8	0	1.118883	-0.139609	0.714229
21	6	0	2.027684	-0.878934	0.100912
22	8	0	1.944389	-2.006349	-0.221304
23	6	0	3.279324	-0.023923	-0.132180
24	9	0	4.148328	-0.692458	-0.844320
25	9	0	2.972371	1.084898	-0.764506
26	9	0	3.825105	0.286024	1.024181
27	9	0	-0.466948	1.817946	-1.078674
28	9	0	-1.974683	2.815963	0.043821
29	9	0	-0.256842	2.070297	1.032220

CP7

E(MP2/6-31G**//HF/6-31G*) = -1245.5834780281 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.634881	0.436104	0.251564
2	6	0	2.543547	-1.285789	-0.179876
3	6	0	2.974345	0.915223	1.035218
4	6	0	3.173738	1.889944	-0.129123
5	6	0	1.841051	2.498420	-0.568860
6	6	0	0.804674	1.420143	-0.900064
7	8	0	0.051760	1.122411	1.296113
8	1	0	-0.157908	1.873400	-1.095870
9	1	0	1.454082	3.134345	0.220879
10	1	0	1.097339	0.868969	-1.783510
11	1	0	1.984992	3.128359	-1.440762
12	1	0	3.854031	2.675904	0.183815
13	1	0	2.595519	1.461622	1.891116
14	1	0	3.645670	1.384758	-0.965682
15	1	0	3.915589	0.473979	1.334679
16	1	0	-0.182728	0.518476	1.993209
17	6	0	1.960794	-0.207810	0.728400
18	1	0	1.742262	-0.738242	1.650089
19	8	0	-0.186611	-0.667362	-0.106640
20	8	0	-1.427399	-0.218620	-0.519752
21	6	0	-2.354212	-0.392548	0.411740
22	8	0	-2.208574	-0.768603	1.513909
23	6	0	-3.717260	-0.023267	-0.185373
24	9	0	-4.642130	-0.089928	0.734616
25	9	0	-4.020761	-0.854531	-1.158147
26	9	0	-3.687012	1.198780	-0.671892
27	9	0	1.818840	-2.388497	-0.172597
28	9	0	3.754340	-1.628657	0.240953
29	9	0	2.670990	-0.906801	-1.443906

CP8

E(MP2/6-31G**//HF/6-31G*) = -1245.5858511725 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.800300	-0.825782	-0.137268
2	6	0	1.768501	1.568136	-0.165439
3	6	0	2.626662	-0.185711	1.468607
4	6	0	3.646554	-0.955456	0.622767
5	6	0	2.980100	-2.095085	-0.150798
6	6	0	1.804540	-1.594691	-0.995825
7	8	0	0.207161	-1.631918	0.810947
8	1	0	1.278861	-2.426155	-1.456216
9	1	0	2.626637	-2.847375	0.547830
10	1	0	2.154453	-0.957836	-1.796560

11	1	0	3.700211	-2.581631	-0.800570
12	1	0	4.414226	-1.356776	1.277062
13	1	0	2.232439	-0.842535	2.234800
14	1	0	4.146173	-0.284654	-0.067873
15	1	0	3.101634	0.642417	1.978367
16	1	0	-0.186390	-2.387595	0.387302
17	6	0	1.419904	0.338204	0.660267
18	1	0	0.664769	0.683762	1.355234
19	8	0	-0.173370	-0.403919	-1.083571
20	8	0	-1.233523	0.208543	-0.440440
21	6	0	-2.283628	-0.592836	-0.340933
22	8	0	-2.361212	-1.724586	-0.642748
23	6	0	-3.452263	0.209162	0.244143
24	9	0	-4.475726	-0.576788	0.449632
25	9	0	-3.103000	0.760443	1.386527
26	9	0	-3.805960	1.161409	-0.590789
27	9	0	0.700195	2.157099	-0.667694
28	9	0	2.374640	2.468218	0.597818
29	9	0	2.586575	1.316038	-1.180606

TS1

E(MP2/6-31G**//HF/6-31G*) = -1245.5481623199 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.839981	0.702531	0.842742
2	1	0	1.800265	2.305012	1.817426
3	6	0	1.810276	2.768610	-0.305853
4	6	0	3.132392	2.087219	-0.656054
5	6	0	2.950261	0.602775	-0.975360
6	6	0	2.262013	-0.157451	0.144326
7	8	0	0.350939	0.228570	-0.251416
8	6	0	2.099330	-1.643287	-0.129425
9	1	0	2.381829	0.481028	-1.888116
10	1	0	2.778697	-0.070888	1.092931
11	1	0	3.918642	0.136424	-1.133388
12	1	0	3.583031	2.571928	-1.515168
13	1	0	1.118522	2.692648	-1.138346
14	1	0	3.832488	2.201225	0.169217
15	1	0	1.977391	3.825938	-0.130856
16	8	0	-1.413827	0.777354	-0.367992
17	6	0	1.170827	2.172561	0.944416
18	6	0	-2.147677	-0.073976	0.203405
19	1	0	0.219972	2.648114	1.162492
20	8	0	0.448964	0.171494	1.983931
21	1	0	-0.277657	-0.454825	1.821020
22	8	0	-1.852457	-0.870584	1.062656
23	6	0	-3.598965	-0.034869	-0.302996
24	9	0	-3.637500	-0.326706	-1.589920

25	9	0	-4.366408	-0.888139	0.333176
26	9	0	-4.108975	1.172964	-0.142107
27	9	0	1.611950	-1.892456	-1.324018
28	9	0	1.340710	-2.238758	0.762759
29	9	0	3.303250	-2.197566	-0.069429

TS2

E(MP2/6-31G**//HF/6-31G*) = -1245.5459474795 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.095973	-0.642493	0.704409
2	1	0	-2.752077	0.585504	1.060477
3	6	0	-2.787700	0.133555	-1.055016
4	6	0	-3.660911	-1.114037	-0.934072
5	6	0	-2.833620	-2.362090	-0.630142
6	6	0	-1.980803	-2.188300	0.603582
7	8	0	-0.366267	-1.271018	-0.143867
8	1	0	-1.303195	-2.995323	0.822070
9	1	0	-2.205644	-2.617414	-1.475114
10	1	0	-2.540971	-1.941888	1.497018
11	1	0	-3.488093	-3.211938	-0.450197
12	1	0	-4.205423	-1.261483	-1.860093
13	1	0	-2.065437	0.006888	-1.852688
14	1	0	-4.405191	-0.968114	-0.153891
15	1	0	-3.405206	0.984108	-1.316788
16	8	0	1.108484	-0.230893	-0.607523
17	6	0	-2.044622	0.465434	0.247702
18	6	0	2.029377	-0.421225	0.225859
19	6	0	-1.369962	1.833298	0.120356
20	8	0	-0.637598	-0.493914	1.937239
21	1	0	0.316725	-0.702439	1.954084
22	8	0	1.947185	-0.811346	1.369951
23	6	0	3.422852	-0.110085	-0.344978
24	9	0	3.701151	-0.953416	-1.323735
25	9	0	4.363376	-0.217160	0.564472
26	9	0	3.464152	1.113475	-0.834987
27	9	0	-0.719940	1.971061	-1.015439
28	9	0	-2.318511	2.764295	0.141017
29	9	0	-0.538199	2.101203	1.102286

TS3

E(MP2/6-31G**//HF/6-31G*) = -1245.5426490741 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.658571	0.129451	-0.517149

2	1	0	1.766678	1.008857	-2.079941
3	6	0	1.556433	2.532173	-0.547665
4	6	0	2.788574	2.189151	0.285944
5	6	0	2.472608	1.135128	1.348190
6	6	0	1.895767	-0.175765	0.825312
7	8	0	-0.006041	0.282411	0.575728
8	1	0	1.477548	-0.764954	1.623986
9	1	0	1.754600	1.538960	2.051049
10	6	0	2.886277	-1.111507	0.124866
11	1	0	3.363845	0.890361	1.915392
12	1	0	3.149993	3.077568	0.792710
13	1	0	0.765879	2.907017	0.094709
14	1	0	3.592576	1.849199	-0.359549
15	1	0	1.793520	3.325141	-1.248831
16	8	0	-1.755025	0.753231	0.090018
17	6	0	1.047252	1.335251	-1.342219
18	6	0	-2.429493	-0.303051	-0.020184
19	1	0	0.132872	1.583690	-1.872043
20	8	0	0.399332	-0.936785	-1.243516
21	1	0	-0.377437	-1.399604	-0.881095
22	8	0	-2.042693	-1.428197	-0.242571
23	6	0	-3.937507	-0.065780	0.164619
24	9	0	-4.177358	0.371216	1.388034
25	9	0	-4.637131	-1.160307	-0.022015
26	9	0	-4.369617	0.846149	-0.686902
27	9	0	3.308134	-0.670416	-1.042680
28	9	0	2.392832	-2.315448	-0.035391
29	9	0	3.948078	-1.223619	0.909626

TS4

E(MP2/6-31G**//HF/6-31G*) = -1245.5499509937 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739563	0.245986	-0.595412
2	6	0	2.579892	-1.332263	0.152201
3	6	0	2.029184	0.752733	1.539334
4	6	0	2.936833	1.789595	0.872997
5	6	0	2.210432	2.561406	-0.230931
6	6	0	1.577954	1.655356	-1.263977
7	8	0	-0.120834	1.158104	-0.322850
8	1	0	0.936402	2.145397	-1.976056
9	1	0	1.450765	3.203696	0.198231
10	1	0	2.277868	1.021166	-1.790170
11	1	0	2.911147	3.205091	-0.757422
12	1	0	3.278863	2.491993	1.625249
13	1	0	1.163163	1.246756	1.964236
14	1	0	3.823116	1.311452	0.469400
15	1	0	2.547840	0.274176	2.358715

16	8	0	-1.552583	0.366976	0.570008
17	6	0	1.509747	-0.337580	0.587137
18	6	0	-2.395424	-0.030775	-0.276888
19	1	0	0.764991	-0.928078	1.111415
20	8	0	0.447419	-0.613617	-1.561565
21	1	0	-0.498913	-0.539873	-1.781334
22	8	0	-2.220337	-0.317722	-1.438786
23	6	0	-3.813139	-0.144599	0.306696
24	9	0	-4.239293	1.046286	0.686717
25	9	0	-4.668193	-0.626054	-0.564128
26	9	0	-3.814516	-0.936062	1.363308
27	9	0	3.366898	-0.846587	-0.804061
28	9	0	3.363680	-1.641202	1.173251
29	9	0	2.065335	-2.456477	-0.293271

TS5

E(MP2/6-31G**//HF/6-31G*) = -1245.5449234619 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.844267	0.856949	0.010680
2	1	0	-1.338953	2.117805	-1.622742
3	6	0	-2.519668	2.716989	0.099097
4	6	0	-3.667113	1.733512	-0.130055
5	6	0	-3.318922	0.308877	0.305878
6	6	0	-2.149465	-0.312173	-0.480842
7	8	0	-0.626832	0.847916	1.309536
8	6	0	-1.909145	-1.770533	-0.110903
9	1	0	-3.103052	0.266993	1.365628
10	1	0	-2.293916	-0.235542	-1.544734
11	1	0	-4.166506	-0.341377	0.119104
12	1	0	-4.545945	2.052981	0.419475
13	1	0	-2.356214	2.859310	1.161531
14	1	0	-3.942157	1.728440	-1.182606
15	1	0	-2.769042	3.685167	-0.319998
16	1	0	0.137154	0.272775	1.508353
17	6	0	-1.235580	2.203721	-0.547718
18	1	0	-0.394321	2.857083	-0.344821
19	8	0	-0.190684	0.030080	-0.722632
20	8	0	1.586920	0.626113	-0.763840
21	6	0	2.211682	0.109726	0.197532
22	8	0	1.775883	-0.302625	1.249419
23	6	0	3.726314	0.025613	-0.054333
24	9	0	4.372279	-0.469697	0.975313
25	9	0	4.217183	1.226132	-0.305128
26	9	0	3.969834	-0.742079	-1.100249
27	9	0	-1.103719	-2.378023	-0.950630
28	9	0	-3.068258	-2.414197	-0.155103
29	9	0	-1.426472	-1.901201	1.105234

TS6

E(MP2/6-31G**//HF/6-31G*) = -1245.5458984981 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.025104	-0.695399	-0.040776
2	1	0	-2.140572	0.433121	-1.451895
3	6	0	-3.358075	0.168646	0.319775
4	6	0	-3.971328	-1.160103	-0.116002
5	6	0	-3.009742	-2.325334	0.090333
6	6	0	-1.722225	-2.201291	-0.724200
7	8	0	-0.780063	-0.843549	1.249174
8	1	0	-1.032212	-3.001122	-0.522293
9	1	0	-2.766454	-2.446984	1.137634
10	1	0	-1.900165	-2.082478	-1.779123
11	1	0	-3.463375	-3.254985	-0.247515
12	1	0	-4.878878	-1.340119	0.449639
13	1	0	-3.206742	0.177368	1.392686
14	1	0	-4.259941	-1.106681	-1.163508
15	1	0	-4.033193	0.978754	0.079869
16	1	0	0.161507	-1.083295	1.374936
17	6	0	-2.010262	0.425750	-0.375978
18	6	0	-1.494058	1.817355	-0.024259
19	8	0	-0.109091	-1.042745	-0.874351
20	8	0	1.407879	0.037389	-0.737500
21	6	0	2.150514	-0.423753	0.161054
22	8	0	1.850863	-1.107896	1.117787
23	6	0	3.629043	-0.047329	-0.032644
24	9	0	4.375375	-0.445801	0.971423
25	9	0	3.767053	1.258596	-0.151982
26	9	0	4.090809	-0.611092	-1.135088
27	9	0	-1.258172	1.963626	1.263647
28	9	0	-2.415631	2.712957	-0.361158
29	9	0	-0.400465	2.125001	-0.681857

TS7

E(MP2/6-31G**//HF/6-31G*) = -1245.5449895476 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.669200	-0.806202	-0.098896
2	1	0	-1.402503	-0.810258	1.889611
3	6	0	-2.423803	-2.374422	0.784805
4	6	0	-3.535844	-1.512354	0.185834
5	6	0	-3.045763	-0.728545	-1.033996
6	6	0	-1.928505	0.305327	-0.778322

7	8	0	-0.253729	-1.592394	-1.077187
8	1	0	-1.512972	0.647409	-1.710488
9	1	0	-2.681886	-1.411587	-1.789453
10	6	0	-2.362780	1.520156	0.032005
11	1	0	-3.860050	-0.165632	-1.477041
12	1	0	-4.358848	-2.143509	-0.131968
13	1	0	-2.149582	-3.159059	0.087524
14	1	0	-3.932616	-0.835891	0.935264
15	1	0	-2.772695	-2.858600	1.689825
16	1	0	0.584281	-1.240357	-1.437870
17	6	0	-1.191059	-1.533784	1.116487
18	1	0	-0.368442	-2.155597	1.451717
19	8	0	-0.095035	0.335990	0.031751
20	8	0	1.619501	0.013046	0.714502
21	6	0	2.410337	-0.150830	-0.247673
22	8	0	2.163288	-0.520593	-1.375571
23	6	0	3.869088	0.171771	0.116057
24	9	0	4.690062	-0.063590	-0.880840
25	9	0	4.257851	-0.556657	1.146338
26	9	0	3.980345	1.444331	0.448380
27	9	0	-2.511948	1.258733	1.316875
28	9	0	-3.534442	1.941490	-0.422550
29	9	0	-1.520950	2.519916	-0.087414

TS8

E(MP2/6-31G**//HF/6-31G*) = -1245.5483340034 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.900628	-0.906614	-0.085673
2	6	0	-1.627847	1.588902	-0.186785
3	6	0	-2.718085	-0.052342	1.418926
4	6	0	-3.775686	-0.724927	0.535671
5	6	0	-3.196079	-1.924268	-0.218524
6	6	0	-1.935761	-1.548559	-1.004786
7	8	0	-0.534282	-1.852385	0.862685
8	1	0	-1.477001	-2.429671	-1.436378
9	1	0	-2.952076	-2.714555	0.483208
10	1	0	-2.175847	-0.865821	-1.808421
11	1	0	-3.933071	-2.326124	-0.906250
12	1	0	-4.598522	-1.050812	1.164522
13	1	0	-2.425005	-0.738040	2.204540
14	1	0	-4.187231	-0.010169	-0.168202
15	1	0	-3.127805	0.825067	1.902795
16	1	0	0.399724	-1.852724	1.016947
17	6	0	-1.429600	0.339354	0.660909
18	1	0	-0.680948	0.626911	1.389421
19	8	0	0.183326	-0.622128	-0.951603
20	8	0	1.208459	0.012270	-0.257489

21	6	0	2.335551	-0.691983	-0.280023
22	8	0	2.471340	-1.814960	-0.586457
23	6	0	3.480221	0.206727	0.203262
24	9	0	4.579971	-0.489266	0.309327
25	9	0	3.185591	0.719804	1.380016
26	9	0	3.672239	1.187924	-0.647777
27	9	0	-0.498578	2.040055	-0.700473
28	9	0	-2.119713	2.566471	0.563929
29	9	0	-2.471229	1.423436	-1.198034