Electronic Supplementary Information

Pentalenene Formation Mechanisms Redux

Michael W. Lodewyk, Dan Willenbring, and Dean J. Tantillo

Contents

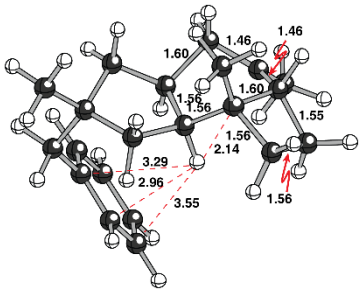
Full *GAUSSIAN03* and *GAUSSIAN09* References

GAUSSIAN03, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, **2004**.

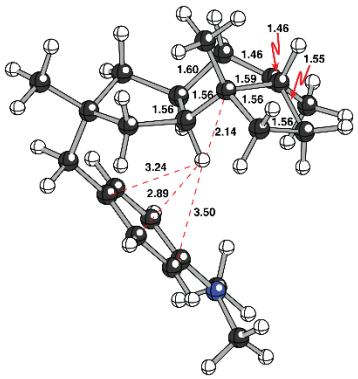
GAUSSIAN09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

Benzyl Analogs of Cation C (reactants for TSS in manuscript)

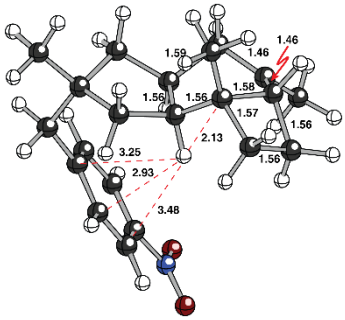
See Coordinates and Energies section for B3LYP free energies and M06-2X single point energies



SI-1
X=H



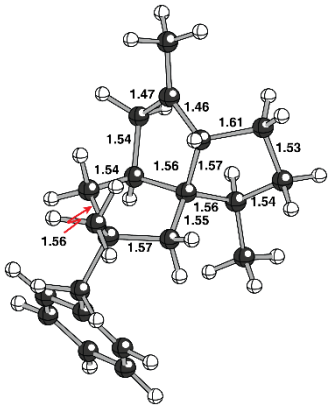
SI-2
X=NMe_2



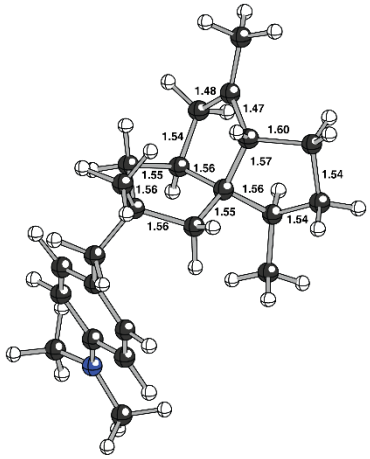
SI-3
X=NO_2

Benzyl Analogs of Cation F (products for TSS in manuscript)

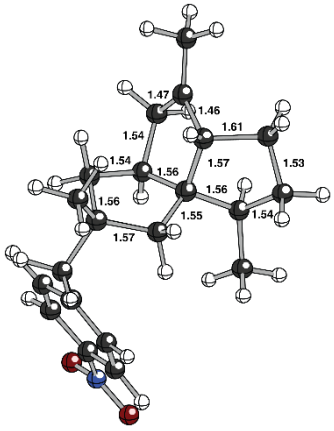
See Coordinates and Energies section for B3LYP free energies and M06-2X single point energies



SI-4
X=H



SI-5
X=NMe_2

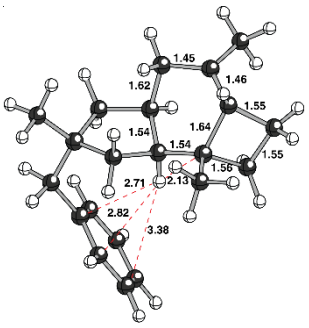
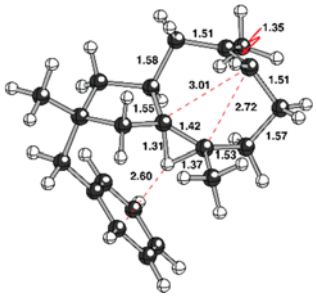
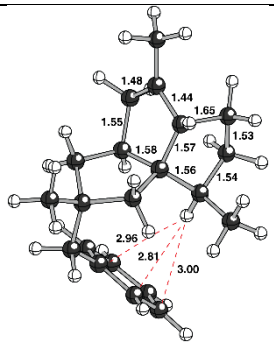
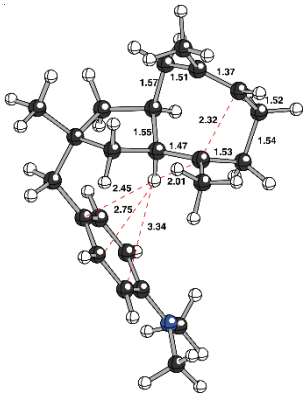
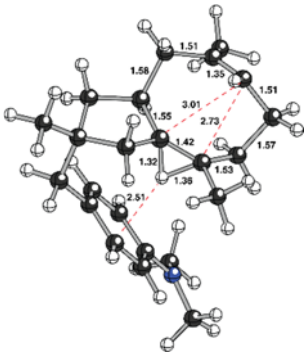
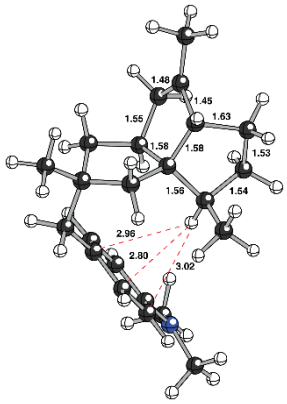
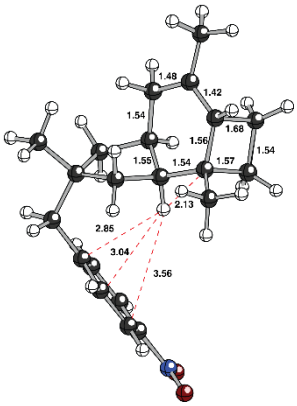
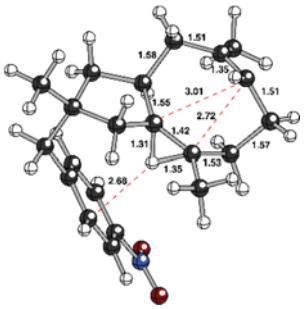
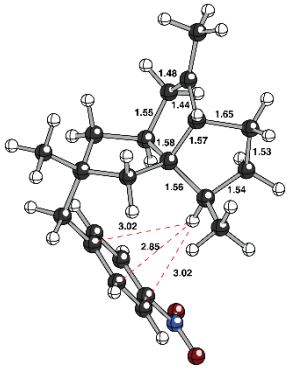


SI-6
X=NO_2

Benzyl Analogs of Cation C', TS(C'→F'), and Cation F'

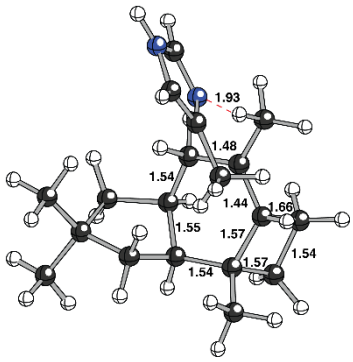
B3LYP free energies in kcal/mol relative to each reactant.

Reactants for NMe_2 and NO_2 analogs optimize to a lower energy conformer, resulting in higher barriers.

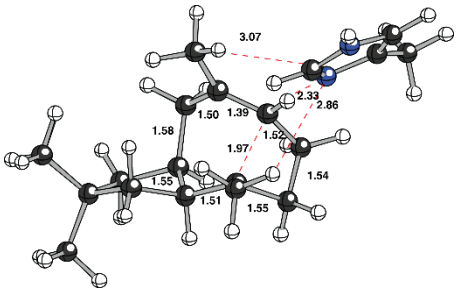
		
SI-7 **C' (X=H)** "0" kcal/mol	**SI-8** **TS(C'→F') (X=H)** 15.10	**SI-9** **F' (X=H)** -13.32
		
SI-10 **C' (X=NMe_2)** "0" kcal/mol	**SI-11** **TS(C'→F') (X=NMe_2)** 18.08	**SI-12** **F' (X=NMe_2)** -9.47
		
SI-13 **C' (X=NO_2)** "0" kcal/mol	**SI-14** **TS(C'→F') (X=NO_2)** 21.51	**SI-15** **F' (X=NO_2)** -9.62

Additional 4-methylimidazole complexes with cation C'

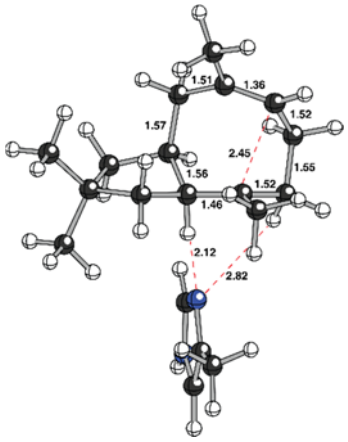
B3LYP free energies in kcal/mol relative to cation C (4-methylimidazole complex) in manuscript.



SI-16
-8.38



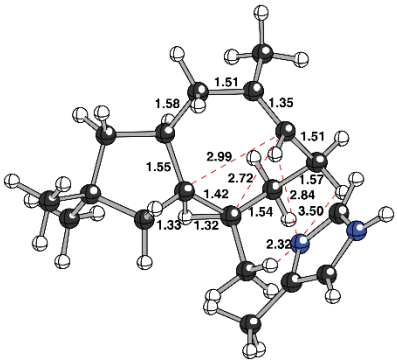
SI-17
-6.47



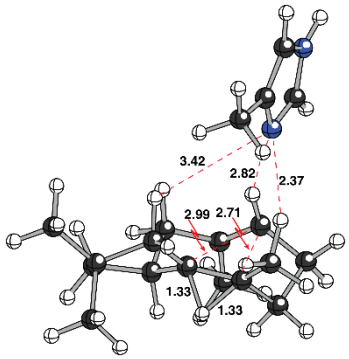
SI-18
-7.08

Additional 4-methylimidazole complexes with TS(C'→F')

B3LYP free energies in kcal/mol relative to TS(C→F) (4-methylimidazole complex) in manuscript.



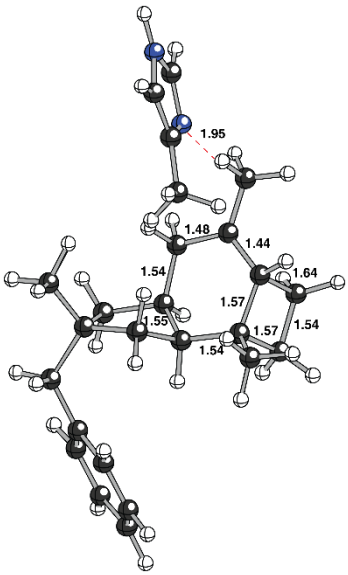
SI-19
-11.05



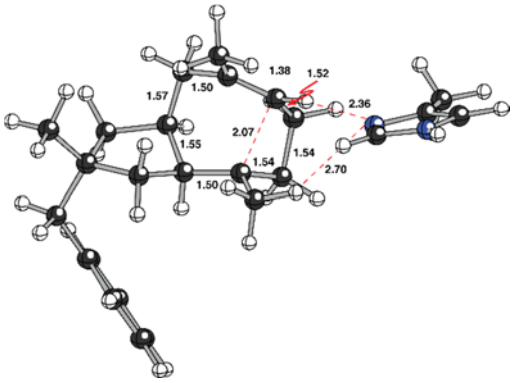
SI-20
-11.60

Additional 4-methylimidazole complexes with benzyl analogs of cation C'

B3LYP free energies in kcal/mol relative to cation C (Bn Analog/4-methylimidazole complex) in manuscript.



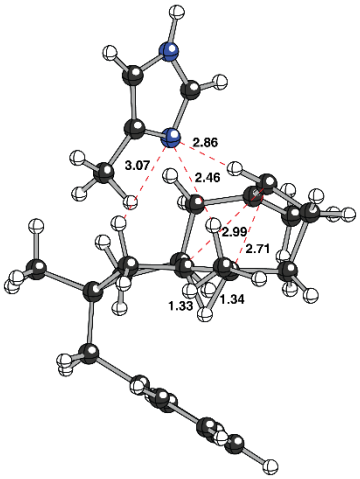
SI-21
-9.36



SI-22
-7.84

Additional 4-methylimidazole complex with benzyl analog of TS(C'→F')

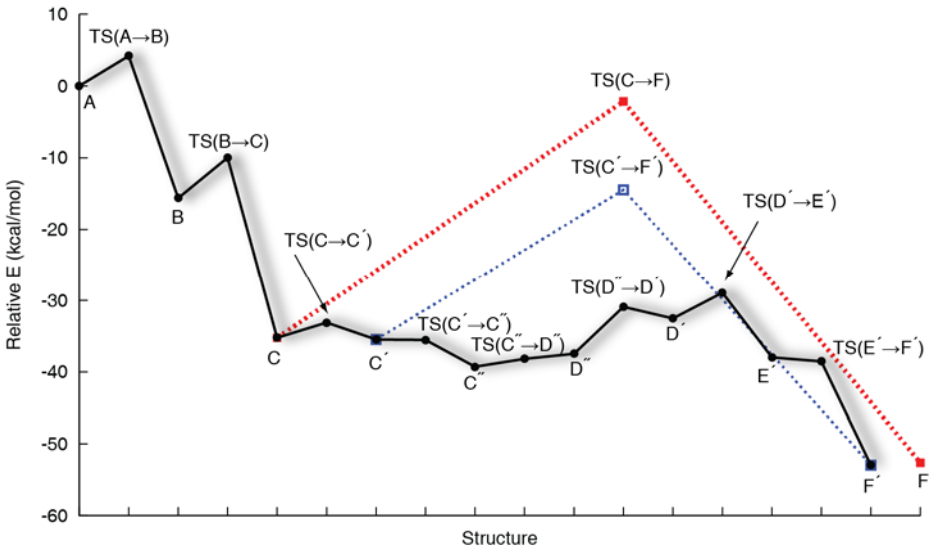
B3LYP free energies in kcal/mol relative to TS(C→F) (Bn Analog/4-methylimidazole complex) in manuscript.



SI-23
-21.78

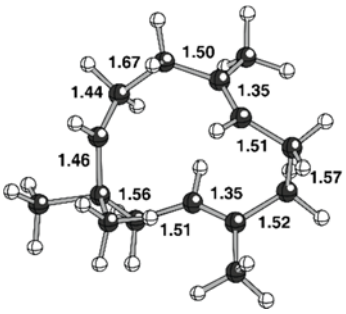
mPW1PW91 Single Point Energy Plot

Plot corresponding to Fig. 12 in the manuscript, with mPW1PW91 electronic energies (with unscaled B3LYP zero-point energy corrections added).

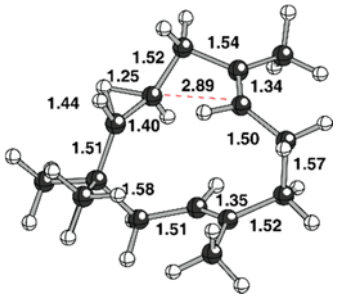


Initial Pathway Structures (Cation A through TS(B→C); not shown in manuscript; from P. Gutta and D. J. Tantillo, *J. Am. Chem. Soc.*, **2006**, *128*, 6172–6179.**)**

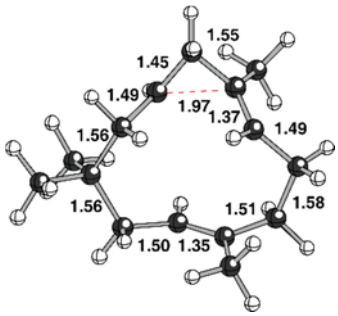
See Coordinates and Energies section for B3LYP free energies and mPW1PW91 single point energies.



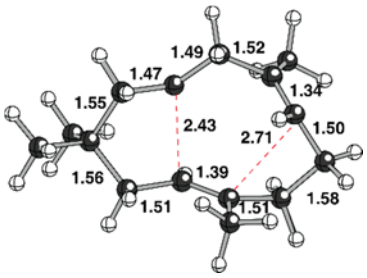
Cation A



TS(A→B)

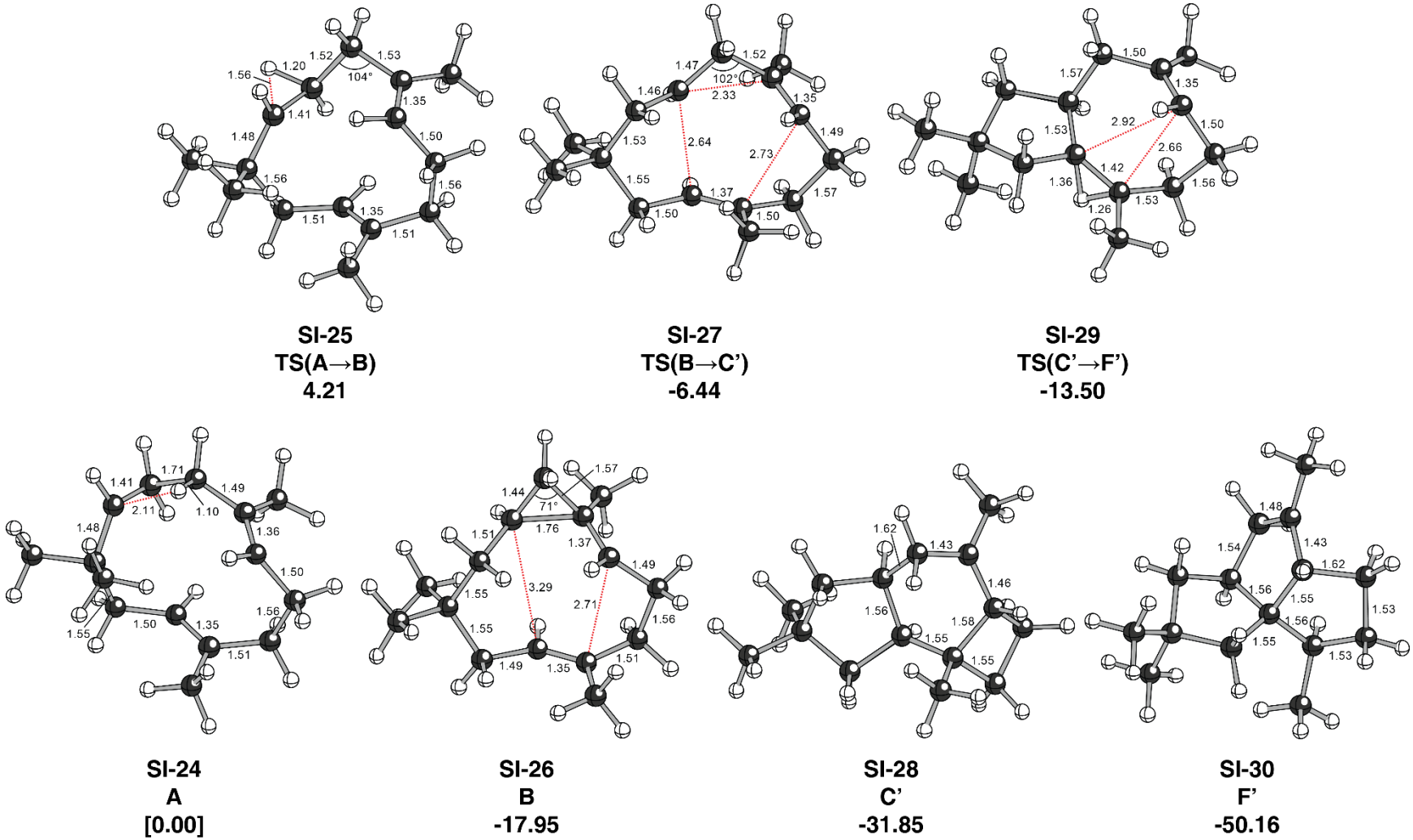


Cation B



TS(B→C)

MP2 Pathway

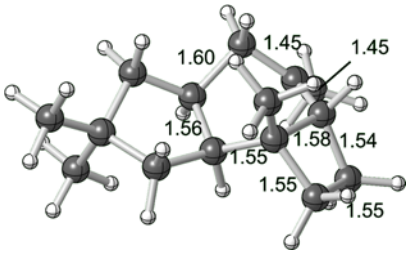


MP2/6-31+G(d,p) computed structures and free energies relative to Cation A, for Path A in manuscript Figure 1.

Re-optimization of Cation C, TS(C→F), and Cation F with M06-2X/6-31+G(d,p)

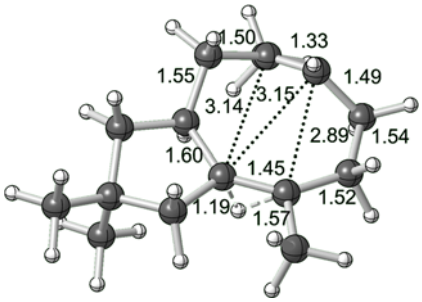
In addition to the M06-2X/6-31+G(d,p) single-point calculations discussed in the manuscript, Cation C, TS(C→F), and Cation F were re-optimized at this level of theory. Re-optimization of these structures resulted in slight geometrical changes in these structures compared to the B3LYP/6-31+G(d,p) structures. Most notably, the transition state structure appears to be somewhat earlier with respect to hydrogen atom migration. The relative energies of the transition state structure and product cation are very close to those computed with the B3LYP method.

Shown here are the computed structures, and free energies relative to cation C, along with the B3LYP relative free energies.



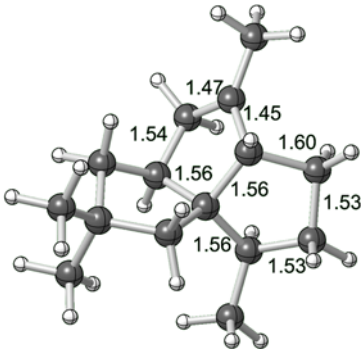
SI-31

“0” kcal/mol



SI-32

30.51



SI-33

-17.53

B3LYP/6-31+G(d,p) computed free energies:

“0”	30.36	-15.93

Coordinates and Energies for all Structures in Manuscript and ESI

Cation A

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.0494640 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.364004 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2301285 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.252808	0.874856	1.359109
2	1	2.841119	1.779050	1.182616
3	1	1.255413	1.171165	1.688914
4	1	2.734403	0.309743	2.162904
5	6	2.170796	0.059468	0.041802
6	6	1.705979	-1.297628	0.311392
7	6	0.804367	-2.180111	-0.378614
8	1	1.269554	-3.170116	-0.457324
9	6	-0.498235	-2.461103	0.621686
10	1	-0.729248	-3.510899	0.427877
11	6	-1.653524	-1.556786	0.315496
12	6	-1.800409	-0.421891	1.028106
13	6	-2.743795	0.723223	0.765118
14	1	-3.763899	0.372438	0.575817
15	1	-2.793985	1.355816	1.656423
16	6	-2.288686	1.581728	-0.466676
17	6	-0.793683	1.857710	-0.479376
18	6	1.512103	0.865786	-1.116989
19	1	1.975816	1.857880	-1.099982
20	1	1.812096	0.412891	-2.069494
21	6	-2.536431	-1.970165	-0.836106
22	1	-2.943744	-2.974462	-0.669814
23	1	-3.377923	-1.290054	-0.976499
24	1	-1.982834	-2.009264	-1.784507
25	1	2.164875	-1.740942	1.200087
26	6	3.673790	-0.310647	-0.380504
27	1	4.136602	0.653749	-0.615196
28	1	3.714381	-0.938840	-1.273209
29	1	4.236686	-0.776961	0.430591
30	1	-1.077005	-0.249307	1.826306
31	1	-0.168932	-2.378817	1.659786
32	1	0.458269	-1.829898	-1.348611
33	6	0.005805	0.955105	-1.078886
34	1	-0.499906	0.152616	-1.610492
35	6	-0.334066	3.100598	0.237133
36	1	-0.814656	3.981708	-0.204658
37	1	-0.631564	3.088192	1.294034
38	1	0.745936	3.253885	0.191833
39	1	-2.860575	2.515935	-0.463967
40	1	-2.561795	1.043640	-1.379580

TS(A→B)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.0383850 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.361589 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2210695 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.685396	0.428530	1.264900
2	1	3.468088	1.140639	0.990701
3	1	1.846191	0.993921	1.676503
4	1	3.085305	-0.222967	2.048598
5	6	2.279702	-0.387271	0.005599
6	6	1.217913	-1.340583	0.495699
7	6	0.138118	-1.906193	-0.202301
8	1	1.133226	-2.651583	-0.096305
9	6	-1.113575	-2.438508	0.467400
10	1	-1.462566	-3.348310	-0.026301
11	6	-2.124988	-1.289018	0.281105
12	6	-1.860499	-0.118417	0.885208
13	6	-2.502713	1.226977	0.681612
14	1	-3.569313	1.144066	0.453214
15	1	-2.423818	1.807675	1.606614
16	6	-1.812624	2.008887	-0.493887
17	6	-0.292723	1.968303	-0.445290
18	6	1.789090	0.572127	-1.149598
19	1	2.459581	1.437634	-1.117597
20	1	1.988993	0.081032	-2.108699
21	6	-3.257987	-1.555728	-0.673793
22	1	-3.862077	-2.403435	-0.328194
23	1	-3.918396	-0.693334	-0.778190
24	1	-2.889886	-1.819121	-1.674695
25	1	1.276418	-1.621385	1.550898
26	6	3.517510	-1.195856	-0.475705
27	1	4.303002	-0.492047	-0.765605
28	1	3.278915	-1.812857	-1.348107
29	1	3.919018	-1.838454	0.314192
30	1	-0.981898	-0.089109	1.533006
31	1	-0.929871	-2.667009	1.521899
32	1	0.063514	-1.688491	-1.265200
33	6	0.335386	0.992412	-1.129794
34	1	-0.311409	0.386006	-1.760994
35	6	0.376767	3.009008	0.414711
36	1	0.064656	4.009606	0.092514
37	1	0.077070	2.920602	1.467612
38	1	1.466667	2.970420	0.366709
39	1	-2.175535	3.042583	-0.472884
40	1	-2.154521	1.565886	-1.434888

Cation B

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.068497 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.364782 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2558043 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.651895	0.102213	-0.657405
2	1	-4.310590	0.791420	-0.120607
3	1	-3.502391	0.504410	-1.665806
4	1	-4.177402	-0.854983	-0.747703
5	6	-2.311397	-0.056295	0.094697
6	6	-1.396903	-0.940404	-0.810200
7	6	-0.325110	-1.798711	-0.233896
8	6	0.657185	-2.530620	-1.007293
9	1	0.821277	-3.574121	-0.737791
10	6	1.631692	-1.609626	-0.233194
11	6	1.873402	-0.360529	-0.730097
12	6	2.843409	0.648165	-0.216798
13	1	3.683304	0.180660	0.303204
14	1	3.245914	1.198860	-1.073399
15	6	2.135315	1.666072	0.761399
16	6	0.752119	2.036282	0.270496
17	6	-1.722686	1.375601	0.309695
18	1	-1.812581	1.931699	-0.628707
19	1	-2.379583	1.882808	1.029693
20	6	2.320885	-2.207528	0.968508
21	1	3.188881	-2.791436	0.639111
22	1	2.663590	-1.449129	1.674207
23	1	1.663680	-2.896422	1.507709
24	1	-2.044708	-1.739000	-1.230398
25	6	-2.587104	-0.744690	1.446399
26	1	-3.355000	-0.190883	1.994396
27	1	-1.706805	-0.791895	2.096300
28	1	-2.963612	-1.765587	1.308700
29	1	1.283405	-0.048027	-1.589198
30	1	0.634188	-2.376423	-2.085094
31	1	-0.426913	-2.080808	0.811404
32	6	-0.303187	1.385291	0.793496
33	1	-0.101993	0.742692	1.651498
34	6	0.697728	3.039580	-0.854906
35	1	1.107735	3.999077	-0.516508
36	1	1.311626	2.730773	-1.712105
37	1	-0.313870	3.227786	-1.217408
38	1	2.793522	2.536768	0.851298
39	1	2.069010	1.199075	1.748500
40	1	-1.051397	-0.396109	-1.696700

TS(B→C)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.059676 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.363422 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2454514 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.918111	0.294797	-0.669089
2	1	-4.496513	1.030688	-0.101479
3	1	-3.710114	0.721910	-1.656184
4	1	-4.552608	-0.586604	-0.806899
5	6	-2.622208	-0.061908	0.078604
6	6	-1.766906	-1.019794	-0.797509
7	6	-0.439504	-1.334596	-0.243915
8	6	0.713596	-1.816982	-1.058023
9	1	0.597100	-2.918782	-1.067437
10	6	2.019796	-1.400985	-0.394220
11	6	2.523091	-0.231478	-0.809506
12	6	3.246189	0.768514	0.047205
13	1	4.016691	0.337608	0.691499
14	1	3.726685	1.541823	-0.557386
15	6	2.123688	1.382598	0.968015
16	6	0.795786	1.560702	0.271519
17	6	-1.745813	1.208593	0.266819
18	1	-1.740016	1.773305	-0.669874
19	1	-2.222914	1.855482	1.015828
20	6	2.468700	-2.184399	0.809970
21	1	2.681004	-3.222594	0.526556
22	1	3.379100	-1.772701	1.249373
23	1	1.707702	-2.226711	1.601170
24	1	-2.287703	-1.995895	-0.848220
25	6	-2.980104	-0.703426	1.433797
26	1	-3.599205	-0.017435	2.020006
27	1	-2.107602	-0.948830	2.048092
28	1	-3.557001	-1.623126	1.290986
29	1	2.102788	0.188132	-1.724000
30	1	0.643493	-1.472769	-2.093819
31	6	-0.339811	0.897093	0.709313
32	1	-0.236507	0.396581	1.671006
33	6	0.763781	2.567416	-0.842968
34	1	0.434978	3.533410	-0.432656
35	1	1.751880	2.728225	-1.278768
36	1	0.062680	2.309423	-1.639770
37	1	2.454685	2.367295	1.329827
38	1	1.995592	0.735587	1.839907
39	1	-1.686009	-0.658081	-1.828705
40	1	-0.411202	-1.632809	0.800881

Cation C

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.086151 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366171 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2884495 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.896209	-0.297180	-0.598995
2	1	4.421415	-1.114877	-0.093397
3	1	3.674210	-0.621979	-1.621795
4	1	4.586103	0.551525	-0.656195
5	6	2.616808	0.080010	0.162408
6	6	1.809099	1.170606	-0.592689
7	6	0.389601	1.055696	-0.002787
8	6	-0.726904	1.590090	-1.005685
9	1	-0.600612	2.658691	-1.189983
10	6	-1.982001	1.242180	-0.350684
11	6	-2.256391	-0.181422	-0.234386
12	6	-2.822485	-0.837028	1.065314
13	1	-2.581788	-0.261028	1.962815
14	1	-3.887683	-1.072335	1.071515
15	6	-1.838477	-2.013021	0.810710
16	6	-1.024485	-1.172313	-0.230389
17	6	1.593815	-1.087197	0.196907
18	1	1.630717	-1.603895	-0.766294
19	1	1.834322	-1.827596	0.966605
20	6	-2.841107	2.268073	0.263720
21	1	-3.732304	1.866767	0.746120
22	1	-2.248010	2.832776	1.001520
23	1	-3.112713	3.014473	-0.496379
24	1	2.231593	2.174109	-0.479688
25	6	2.986107	0.543310	1.586208
26	1	3.531213	-0.245987	2.114206
27	1	2.109606	0.794903	2.193810
28	1	3.632601	1.426815	1.553508
29	1	-2.916091	-0.412925	-1.092485
30	1	-0.606602	1.024792	-1.936386
31	6	0.199111	-0.443706	0.420810
32	1	-0.004287	-0.433610	1.498311
33	6	-0.740482	-1.894109	-1.549091
34	1	-0.113976	-2.774605	-1.380394
35	1	-1.672680	-2.247015	-2.002190
36	1	-0.227987	-1.263804	-2.283891
37	1	-2.339072	-2.862323	0.338010
38	1	-1.280574	-2.369319	1.680209
39	1	1.796099	0.933808	-1.664190
40	1	0.325998	1.688694	0.888414

TS(C→C')

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.082 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366745 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2856326 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.912814	-0.405615	-0.637052
2	1	4.405099	-1.258939	-0.157883
3	1	3.677090	-0.689297	-1.668968
4	1	4.636553	0.415773	-0.669482
5	6	2.650450	0.000086	0.137796
6	6	1.894579	1.155285	-0.574038
7	6	0.453770	1.068386	-0.021428
8	6	-0.612045	1.573852	-1.097554
9	1	-0.435273	2.631577	-1.302430
10	6	-1.864522	1.301162	-0.404230
11	6	-2.297635	-0.076048	-0.454028
12	6	-3.216716	-0.750495	0.580922
13	1	-3.628651	-0.100014	1.355453
14	1	-4.047694	-1.289312	0.121768
15	6	-2.042057	-1.658660	1.040345
16	6	-1.074767	-1.123557	-0.068859
17	6	1.574277	-1.115283	0.117152
18	1	1.556497	-1.551672	-0.886138
19	1	1.795712	-1.926913	0.818124
20	6	-2.515815	2.329780	0.430789
21	1	-3.513183	2.515437	-0.002442
22	1	-2.716074	1.964597	1.444607
23	1	-1.967850	3.271999	0.462969
24	1	2.346587	2.136885	-0.401288
25	6	3.036736	0.390904	1.578326
26	1	3.510227	-0.453221	2.090424
27	1	3.752590	1.219535	1.575568
28	1	-2.550106	-0.285499	-1.503465
29	1	-0.486323	0.972209	-2.000984
30	6	0.226076	-0.418414	0.437312
31	1	0.125371	-0.378902	1.527025
32	6	-0.873996	-2.138359	-1.194830
33	1	-0.389825	-1.703648	-2.075557
34	1	-0.252328	-2.968535	-0.845391
35	1	-1.833008	-2.561561	-1.510002
36	1	-2.236631	-2.732158	0.977679
37	1	-1.696477	-1.427354	2.051287
38	1	1.898806	0.974109	-1.655928
39	1	0.365220	1.726826	0.848498
40	1	2.176765	0.699918	2.182812

Cation C’

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.087022 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366456 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.289115 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.646390	0.364914	-1.085006
2	1	4.135460	-0.538319	-1.465361
3	1	3.157159	0.862144	-1.930846
4	1	4.430819	1.031883	-0.711622
5	6	2.641369	0.018002	0.025856
6	6	1.889144	1.294751	0.544237
7	6	0.375795	0.945734	0.571548
8	6	-0.352855	1.655144	-0.688287
9	1	-0.146467	2.725440	-0.679967
10	6	-1.742217	1.322717	-0.443067
11	6	-2.139819	-0.061089	-0.660214
12	6	-3.264748	-0.676449	0.203271
13	1	-3.969505	0.005182	0.682491
14	1	-3.838869	-1.418483	-0.353701
15	6	-2.173268	-1.312808	1.104811
16	6	-1.094274	-1.138038	-0.010489
17	6	1.502045	-0.896346	-0.498417
18	1	1.280726	-0.655859	-1.547010
19	1	1.784560	-1.952391	-0.473820
20	6	-2.650425	2.308394	0.182317
21	1	-3.636437	2.265423	-0.298619
22	1	-2.837309	2.022932	1.228933
23	1	-2.259057	3.325505	0.157178
24	1	2.220255	1.570572	1.550439
25	6	3.386618	-0.663775	1.191502
26	1	3.892617	-1.572863	0.849477
27	1	2.713450	-0.943695	2.009981
28	1	4.148023	0.004637	1.607081
29	1	-2.195148	-0.203344	-1.752243
30	1	0.060374	1.182430	-1.583083
31	6	0.286597	-0.586925	0.401492
32	1	0.493180	-1.023048	1.389887
33	6	-1.006095	-2.397313	-0.877604
34	1	-0.467572	-2.221567	-1.812571
35	1	-0.478234	-3.183468	-0.327143
36	1	-1.998641	-2.784921	-1.124868
37	1	-2.341943	-2.338986	1.441563
38	1	-1.958772	-0.685441	1.977292
39	1	2.087179	2.160997	-0.094405
40	1	-0.101392	1.303762	1.489230

TS(C'→C")

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.084447 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366338 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2891035 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.627040	0.402432	-1.095084
2	1	4.113276	-0.488504	-1.506689
3	1	3.122638	0.919492	-1.919927
4	1	4.414738	1.062856	-0.716990
5	6	2.640784	0.022842	0.022034
6	6	1.887445	1.282040	0.581342
7	6	0.374752	0.933284	0.595364
8	6	-0.348115	1.659369	-0.655738
9	1	-0.143962	2.729972	-0.635322
10	6	-1.742598	1.325115	-0.438433
11	6	-2.133909	-0.061822	-0.651315
12	6	-3.260993	-0.676250	0.212018
13	1	-3.956721	0.007229	0.701619
14	1	-3.843952	-1.409183	-0.347776
15	6	-2.168509	-1.326316	1.102337
16	6	-1.092162	-1.142471	-0.014634
17	6	1.501267	-0.889126	-0.507347
18	1	1.273382	-0.637719	-1.551963
19	1	1.787766	-1.944334	-0.497279
20	6	-2.669302	2.314458	0.152020
21	1	-3.668604	2.216530	-0.288935
22	1	-2.807302	2.081001	1.220260
23	1	-2.308109	3.339636	0.065667
24	1	2.216136	1.521602	1.597614
25	6	3.407467	-0.680378	1.160674
26	1	3.918027	-1.575443	0.789597
27	1	4.167491	-0.015245	1.584036
28	1	-2.199742	-0.195820	-1.744674
29	1	0.073080	1.199585	-1.554135
30	6	0.288966	-0.596338	0.402317
31	1	0.500123	-1.047713	1.382953
32	6	-1.004565	-2.396280	-0.890048
33	1	-0.467481	-2.214019	-1.824661
34	1	-0.476020	-3.186427	-0.346120
35	1	-1.997633	-2.781921	-1.138767
36	1	-2.339897	-2.355813	1.427290
37	1	-1.949642	-0.709659	1.981279
38	1	2.087596	2.170575	-0.025324
39	1	-0.107436	1.277913	1.515669
40	1	2.746837	-0.987947	1.979536

Cation C”

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.091425 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366927 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.295644 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.150603	1.185791	-0.958695
2	1	3.535442	0.763650	-1.893570
3	1	2.426104	1.966472	-1.223566
4	1	3.986563	1.673805	-0.446171
5	6	2.522772	0.091266	-0.077176
6	6	1.869961	0.686037	1.224896
7	6	0.350118	0.431334	1.120393
8	6	-0.368867	1.610403	0.430581
9	1	-0.502413	2.462293	1.108823
10	6	-1.625438	1.316426	-0.297361
11	6	-2.015338	-0.023421	-0.565239
12	6	-2.874149	-0.256714	0.855984
13	1	-2.692361	0.477382	1.643320
14	1	-3.939534	-0.284135	0.627930
15	6	-2.100350	-1.580095	1.007245
16	6	-1.140514	-1.256071	-0.187619
17	6	1.338499	-0.617798	-0.810397
18	1	0.936050	0.027254	-1.605049
19	1	1.660717	-1.541759	-1.298199
20	6	-2.480971	2.443876	-0.752724
21	1	-3.472015	2.120604	-1.077293
22	1	-2.560189	3.235460	-0.002001
23	1	-1.980540	2.892929	-1.625471
24	1	2.258970	0.172771	2.109845
25	6	3.609409	-0.935536	0.297900
26	1	4.084499	-1.349752	-0.597969
27	1	4.392799	-0.469754	0.905703
28	1	-2.702175	-0.148902	-1.403801
29	1	0.268528	2.019173	-0.377128
30	6	0.273386	-0.865479	0.278687
31	1	0.627738	-1.687468	0.915668
32	6	-1.136769	-2.331789	-1.274902
33	1	-0.621601	-1.994548	-2.179076
34	1	-0.629838	-3.232028	-0.911371
35	1	-2.156724	-2.617227	-1.553969
36	1	-2.737684	-2.445635	0.810873
37	1	-1.617353	-1.709212	1.978681
38	1	2.103086	1.748821	1.356032
39	1	-0.097868	0.300471	2.112509
40	1	3.195704	-1.770043	0.875823

TS(C"→D")

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.089597 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366225 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2931957 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.151828	1.111276	0.663199
2	1	-3.473235	0.915589	1.692187
3	1	-2.507543	1.999137	0.680873
4	1	-4.044419	1.363316	0.080850
5	6	-2.431091	-0.111857	0.069522
6	6	-1.873321	0.172310	-1.373522
7	6	-0.333480	0.097600	-1.281926
8	6	0.271187	1.497393	-0.920239
9	1	0.740070	1.917572	-1.830391
10	6	1.339185	1.510815	0.097467
11	6	2.187116	0.373343	0.247047
12	6	2.856465	-0.272640	-1.040320
13	1	2.499074	0.183347	-1.964664
14	1	3.942247	-0.172786	-0.994063
15	6	2.274076	-1.664885	-0.755264
16	6	1.340670	-1.078501	0.336389
17	6	-1.161640	-0.480450	0.901789
18	1	-0.808719	0.395803	1.466784
19	1	-1.369998	-1.257671	1.642631
20	6	1.466199	2.685956	0.990393
21	1	2.472519	2.801637	1.398078
22	1	1.130055	3.607162	0.504756
23	1	0.783734	2.526723	1.843029
24	1	-2.225103	-0.593784	-2.072176
25	6	-3.408782	-1.302859	0.031051
26	1	-3.815219	-1.511334	1.026553
27	1	-4.251979	-1.092304	-0.635652
28	1	2.894811	0.474148	1.070389
29	1	-0.497490	2.228959	-0.650202
30	6	-0.106280	-0.914671	-0.131504
31	1	-0.393398	-1.902678	-0.520951
32	6	1.496029	-1.693762	1.720381
33	1	0.989509	-1.113040	2.495973
34	1	1.058691	-2.700156	1.709699
35	1	2.549627	-1.798572	1.995237
36	1	3.008870	-2.363457	-0.348381
37	1	1.766527	-2.149641	-1.592629
38	1	-2.217610	1.133013	-1.771539
39	1	0.103833	-0.249734	-2.221849
40	1	-2.921876	-2.215654	-0.331324

Cation D”

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.091727 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.367208 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2930655 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.247250	1.097204	0.559197
2	1	-3.597287	0.936258	1.584829
3	1	-2.640878	2.010801	0.552106
4	1	-4.127793	1.280040	-0.065536
5	6	-2.454547	-0.117902	0.048316
6	6	-1.863420	0.126026	-1.389372
7	6	-0.325309	0.041959	-1.276793
8	6	0.333494	1.454977	-1.039327
9	1	0.768023	1.785165	-1.993347
10	6	1.406161	1.456851	0.000891
11	6	2.443445	0.536370	-0.023829
12	6	2.839042	-0.382007	-1.176159
13	1	2.366707	-0.097103	-2.117685
14	1	3.920169	-0.397748	-1.327116
15	6	2.259860	-1.681095	-0.585342
16	6	1.306982	-1.033052	0.440080
17	6	-1.201469	-0.388222	0.939850
18	1	-0.884084	0.534223	1.440908
19	1	-1.411356	-1.118668	1.726954
20	6	1.313850	2.449949	1.114368
21	1	2.018069	2.252672	1.925271
22	1	1.562699	3.436524	0.693615
23	1	0.298217	2.538867	1.510751
24	1	-2.220488	-0.645206	-2.079517
25	6	-3.375650	-1.354285	0.034896
26	1	-3.799106	-1.540904	1.027602
27	1	-4.208756	-1.208565	-0.660796
28	1	3.174857	0.615373	0.778681
29	1	-0.429760	2.188821	-0.772036
30	6	-0.115187	-0.866106	-0.038322
31	1	-0.375315	-1.889281	-0.362699
32	6	1.522109	-1.354412	1.891393
33	1	1.010988	-0.661426	2.562779
34	1	1.094222	-2.353817	2.065787
35	1	2.581103	-1.408543	2.152549
36	1	3.022728	-2.277269	-0.077929
37	1	1.738167	-2.323999	-1.300623
38	1	-2.182842	1.085417	-1.808753
39	1	0.110200	-0.400035	-2.176329
40	1	-2.841147	-2.259137	-0.278556

TS(D”→D’)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.085839 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.365872 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.281245 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.591960	1.063297	0.793556
2	1	-4.173784	0.484032	1.518737
3	1	-3.046927	1.840744	1.340731
4	1	-4.302618	1.560176	0.124940
5	6	-2.637721	0.157807	-0.000984
6	6	-1.759693	0.972108	-1.006112
7	6	-0.289206	0.462928	-0.949504
8	6	0.653174	1.538803	-0.392224
9	1	0.623323	2.372931	-1.110006
10	6	2.110004	1.247951	-0.086290
11	6	2.854212	0.190295	-0.475845
12	6	2.453000	-1.023913	-1.300261
13	1	1.796393	-0.760391	-2.129995
14	1	3.341089	-1.480777	-1.744715
15	6	1.779519	-2.092061	-0.390868
16	6	0.824703	-1.386250	0.524504
17	6	-1.581635	-0.500307	0.927026
18	1	-1.255738	0.226122	1.680593
19	1	-1.976381	-1.373353	1.458011
20	6	2.753988	2.337302	0.744877
21	1	3.814957	2.147153	0.920097
22	1	2.663822	3.308009	0.242018
23	1	2.256952	2.443429	1.717413
24	1	-2.154667	0.890206	-2.023042
25	6	-3.461526	-0.916956	-0.740603
26	1	-4.022930	-1.535721	-0.032358
27	1	-4.183276	-0.444938	-1.414725
28	1	3.888985	0.180418	-0.136803
29	1	0.207845	1.958763	0.520610
30	6	-0.426946	-0.857385	-0.017392
31	1	-0.763519	-1.613782	-0.741701
32	6	1.100773	-1.372870	1.968350
33	1	0.664057	-0.517246	2.487655
34	1	0.572605	-2.264644	2.362891
35	1	2.157739	-1.497152	2.205576
36	1	2.539349	-2.614779	0.195572
37	1	1.240616	-2.829166	-0.999641
38	1	-1.775510	2.035128	-0.744427
39	1	0.046552	0.146044	-1.935775
40	1	-2.843039	-1.585702	-1.351041

Cation D’

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.089887 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366323 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2842826 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.902872	0.702996	0.754199
2	1	-4.652609	-0.094694	0.783024
3	1	-3.608151	0.928208	1.785288
4	1	-4.387317	1.593894	0.341621
5	6	-2.695353	0.291684	-0.101318
6	6	-1.578865	1.356356	-0.087234
7	6	-0.231897	0.684175	-0.442357
8	6	0.937870	1.383935	0.271313
9	1	0.774376	2.453829	0.080855
10	6	2.395367	1.106357	-0.075808
11	6	2.914745	0.059261	-0.742878
12	6	2.216690	-1.139647	-1.348549
13	1	1.422766	-0.854707	-2.044609
14	1	2.934855	-1.718477	-1.934326
15	6	1.641770	-2.130594	-0.278020
16	6	0.575026	-1.498385	0.530087
17	6	-1.950576	-0.917683	0.521810
18	1	-1.866572	-0.766636	1.602850
19	1	-2.467522	-1.869959	0.362309
20	6	3.315113	2.191069	0.442875
21	1	4.366297	1.949784	0.272102
22	1	3.101361	3.148600	-0.048203
23	1	3.172492	2.352179	1.518913
24	1	-1.772994	2.179102	-0.785477
25	6	-3.165609	-0.014740	-1.537958
26	1	-3.876134	-0.847966	-1.545006
27	1	-3.673873	0.855750	-1.964522
28	1	3.994891	0.057464	-0.872485
29	1	0.817202	1.298480	1.361802
30	6	-0.564799	-0.928358	-0.154511
31	1	-0.636356	-1.369247	-1.151119
32	6	0.767498	-1.425772	1.986632
33	1	0.005687	-0.872463	2.531315
34	1	0.799300	-2.461968	2.364309
35	1	1.772387	-1.031375	2.195679
36	1	2.448987	-2.512768	0.350963
37	1	1.184731	-2.975038	-0.817372
38	1	-1.506309	1.794225	0.916227
39	1	-0.048409	0.712080	-1.518565
40	1	-2.343740	-0.272222	-2.215267

TS(D'→E')

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.081451 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.363823 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2760572 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.652729	-1.213123	0.669103
2	1	4.329360	-0.556807	1.226937
3	1	3.215517	-1.928817	1.373825
4	1	4.258344	-1.776821	-0.047678
5	6	2.566932	-0.407126	-0.057382
6	6	1.564077	-1.315823	-0.823272
7	6	0.151113	-0.656111	-0.736607
8	6	-0.860983	-1.653519	-0.110114
9	1	-0.851880	-2.538608	-0.762432
10	6	-2.305167	-1.273975	0.148572
11	6	-2.971345	-0.215940	-0.342146
12	6	-2.470804	0.889881	-1.243941
13	1	-1.864349	0.522102	-2.073918
14	1	-3.334877	1.366891	-1.717371
15	6	-1.744878	2.004370	-0.472829
16	6	-0.465798	1.713944	0.297286
17	6	1.638268	0.330621	0.942736
18	1	1.365785	-0.338163	1.772659
19	1	2.091436	1.219435	1.383846
20	6	-3.015788	-2.277826	1.030165
21	1	-4.069930	-2.024984	1.162728
22	1	-2.962603	-3.284727	0.597280
23	1	-2.549871	-2.337189	2.021973
24	1	1.871334	-1.467109	-1.861803
25	6	3.225479	0.608990	-1.011596
26	1	3.860290	1.315000	-0.465365
27	1	3.854907	0.092490	-1.742579
28	1	-4.015147	-0.119495	-0.048406
29	1	-0.434463	-2.010392	0.837957
30	6	0.363621	0.574051	0.159693
31	1	0.556819	1.621174	-0.575841
32	6	-0.144615	2.779628	1.321391
33	1	0.909009	2.844286	1.588149
34	1	-0.492766	3.758872	0.985838
35	1	-0.703402	2.524690	2.231054
36	1	-2.428513	2.404628	0.286939
37	1	-1.532799	2.861547	-1.128883
38	1	1.529817	-2.305496	-0.356404
39	1	-0.192407	-0.362876	-1.726684
40	1	2.493342	1.192132	-1.588161

Cation E’

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.095926 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366256 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2929108 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.509953	0.490900	-0.931436
2	1	3.911585	-0.233373	-1.647804
3	1	3.134052	1.352916	-1.493264
4	1	4.342852	0.834358	-0.309520
5	6	2.415543	-0.136203	-0.058165
6	6	1.771211	0.880308	0.918075
7	6	0.333301	0.368235	1.192779
8	6	-0.764285	1.465413	1.246432
9	1	-1.547609	1.210190	1.964078
10	6	-1.352436	1.628028	-0.154251
11	6	-2.353078	0.830555	-0.606933
12	6	-3.113025	-0.224627	0.155645
13	1	-3.769942	0.252951	0.895886
14	1	-3.778740	-0.736728	-0.543902
15	6	-2.243399	-1.276287	0.897799
16	6	-0.985475	-1.642323	0.089580
17	6	1.173278	-0.564980	-0.910531
18	1	0.960057	0.237530	-1.638753
19	1	1.288742	-1.484378	-1.489609
20	6	-0.791378	2.729238	-1.012589
21	1	-1.255038	2.756711	-2.001390
22	1	-0.961709	3.699572	-0.528020
23	1	0.295183	2.643789	-1.141144
24	1	2.343800	0.988947	1.843339
25	6	2.978839	-1.357392	0.694690
26	1	3.331568	-2.122881	-0.004404
27	1	3.828633	-1.059023	1.316312
28	1	-2.683567	0.999984	-1.630671
29	1	-0.313985	2.400487	1.591900
30	6	0.040895	-0.582638	0.039367
31	1	-0.414904	-2.362285	0.726076
32	6	-1.295040	-2.353951	-1.238704
33	1	-0.409032	-2.804503	-1.691124
34	1	-2.014783	-3.156648	-1.060448
35	1	-1.731971	-1.661290	-1.963653
36	1	-2.833841	-2.182483	1.060775
37	1	-1.959183	-0.917428	1.889633
38	1	1.733715	1.869026	0.449073
39	1	0.314166	-0.225159	2.119093
40	1	2.240529	-1.825951	1.356996

TS(E'→F')

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.091198 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.367606 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2951401 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.470197	0.271116	-0.791717
2	1	3.793404	-0.427778	-1.570352
3	1	3.249019	1.231789	-1.270213
4	1	4.316208	0.422049	-0.113235
5	6	2.256040	-0.273363	-0.024518
6	6	1.740735	0.726293	1.045359
7	6	0.233161	0.429517	1.240771
8	6	-0.698907	1.668765	1.259527
9	1	-1.573950	1.516038	1.898068
10	6	-1.079590	1.715712	-0.204277
11	6	-1.934589	0.761838	-0.720802
12	6	-2.987143	-0.017642	0.036766
13	1	-3.565285	0.654894	0.680417
14	1	-3.686679	-0.431932	-0.692667
15	6	-2.350739	-1.154065	0.877612
16	6	-1.066753	-1.589131	0.156482
17	6	1.012537	-0.416569	-0.967005
18	1	1.000874	0.440079	-1.650333
19	1	1.037486	-1.313595	-1.588453
20	6	-0.396020	2.701126	-1.090965
21	1	-0.579042	2.520602	-2.152185
22	1	-0.800788	3.693360	-0.840766
23	1	0.680251	2.764330	-0.900030
24	1	2.291729	0.641664	1.986403
25	6	2.619686	-1.628268	0.615113
26	1	2.880882	-2.366781	-0.150081
27	1	3.486118	-1.514335	1.274154
28	1	-1.998839	0.730408	-1.807020
29	1	-0.188880	2.574438	1.593729
30	6	-0.174219	-0.379539	-0.037184
31	1	-0.472811	-2.206206	0.855656
32	6	-1.345046	-2.429752	-1.099175
33	1	-0.431897	-2.845584	-1.531108
34	1	-1.990929	-3.272076	-0.836729
35	1	-1.851388	-1.852604	-1.879109
36	1	-3.040852	-1.993487	0.994522
37	1	-2.120112	-0.795328	1.884624
38	1	1.885753	1.752673	0.690078
39	1	0.076168	-0.191800	2.129028
40	1	1.807451	-2.047039	1.219682

Cation F'

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.111536 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.366841 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.3173747 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.388392	-1.042122	-0.955218
2	1	-3.897902	-0.339085	-1.623029
3	1	-2.949420	-1.834064	-1.573046
4	1	-4.150991	-1.498888	-0.315447
5	6	-2.320772	-0.325983	-0.114121
6	6	-1.521513	-1.310261	0.771756
7	6	-0.186764	-0.601072	1.094963
8	6	1.023946	-1.561842	1.134376
9	1	1.766477	-1.290814	1.908061
10	6	1.707477	-1.413573	-0.168441
11	6	1.373742	-0.150370	-0.775622
12	6	2.592985	0.774112	-0.183894
13	1	3.438592	0.209380	0.221077
14	1	2.966025	1.322775	-1.051407
15	6	1.905272	1.663146	0.858368
16	6	0.454725	1.838805	0.369735
17	6	-1.194294	0.265135	-1.001741
18	1	-0.994400	-0.438669	-1.820778
19	1	-1.487898	1.205877	-1.472521
20	6	2.594137	-2.429984	-0.752341
21	1	1.920500	-3.145778	-1.258539
22	1	3.267000	-2.031725	-1.514764
23	1	3.135746	-3.006488	0.003368
24	1	-2.062546	-1.610141	1.675245
25	6	-2.997433	0.763228	0.743032
26	1	-3.489187	1.506898	0.106971
27	1	-2.291310	1.294612	1.388755
28	1	-3.763487	0.321468	1.388780
29	1	1.434175	-0.134361	-1.865944
30	1	0.787790	-2.613060	1.345909
31	6	0.070424	0.401917	-0.111041
32	1	-0.187858	2.134436	1.205591
33	6	0.352894	2.925189	-0.713651
34	1	-0.683194	3.117561	-1.001573
35	1	0.761238	3.867574	-0.335784
36	1	0.905012	2.667174	-1.625246
37	1	2.441396	2.613243	0.955511
38	1	1.931828	1.188584	1.845740
39	1	-1.329703	-2.227877	0.196846
40	1	-0.266499	-0.056579	2.039257

TS(C→F)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.037773 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.363293 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.2328312 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.960573	-0.221402	-0.668266
2	1	-4.559833	0.643784	-0.364441
3	1	-3.824273	-0.175492	-1.754406
4	1	-4.543273	-1.120179	-0.442707
5	6	-2.613222	-0.252727	0.066926
6	6	-1.705892	-1.397567	-0.410118
7	6	-0.253925	-1.005460	-0.056511
8	6	0.779306	-1.803081	-0.905215
9	1	0.489387	-2.858244	-0.840796
10	6	2.118969	-1.495035	-0.304099
11	6	2.679999	-0.357887	-0.738168
12	6	3.259958	0.676681	0.163755
13	1	3.413130	0.295828	1.176499
14	1	4.206576	1.121402	-0.165646
15	6	2.211136	1.813245	0.154676
16	6	0.680931	1.660904	0.037566
17	6	-1.743213	0.967114	-0.295050
18	1	-1.819119	1.169784	-1.375055
19	1	-2.063831	1.873741	0.217646
20	6	2.533117	-2.264222	0.922442
21	1	3.424916	-1.852155	1.398815
22	1	1.738624	-2.336054	1.676825
23	1	2.771257	-3.294942	0.631047
24	1	-1.964630	-2.362690	0.035531
25	6	-2.852162	-0.313424	1.589245
26	1	-3.445371	0.543375	1.926144
27	1	-1.920342	-0.319297	2.168609
28	1	-3.401964	-1.221406	1.855346
29	1	2.339268	0.030817	-1.700475
30	1	0.717399	-1.502466	-1.956460
31	6	-0.272838	0.581846	-0.054690
32	1	0.077195	0.984573	1.095321
33	6	0.083341	3.069412	-0.027370
34	1	-0.649361	3.254532	0.761318
35	1	0.861992	3.825147	0.064154
36	1	-0.425691	3.209798	-0.986323
37	1	2.398932	2.418490	-0.746095
38	1	2.380391	2.513469	0.983611
39	1	-1.793139	-1.509003	-1.498652
40	1	-0.077826	-1.283205	0.989460

Cation F

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.11187 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.36642 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.3164008 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.061987	-1.260079	-1.307000
2	1	-3.612283	-0.576246	-1.962207
3	1	-2.430893	-1.894960	-1.939889
4	1	-3.796968	-1.903411	-0.811519
5	6	-2.226798	-0.483237	-0.277019
6	6	-1.384427	-1.429925	0.612907
7	6	-0.227991	-0.563514	1.143246
8	1	-0.537278	-0.010759	2.034320
9	6	1.065969	-1.356695	1.414892
10	1	1.734572	-0.820904	2.119893
11	6	1.802725	-1.359042	0.138650
12	6	1.379675	-0.255804	-0.706220
13	6	2.555571	0.843758	-0.744835
14	1	3.245697	0.720508	0.096779
15	1	3.128775	0.749937	-1.668631
16	6	1.759170	2.143048	-0.594159
17	1	1.314566	2.428036	-1.555692
18	1	2.403916	2.964934	-0.266032
19	6	0.658256	1.806903	0.424620
20	6	0.121549	0.408458	-0.038841
21	6	-1.132556	0.392093	-0.966067
22	1	-0.876044	-0.050464	-1.936201
23	1	-1.507135	1.395165	-1.183247
24	6	2.810527	-2.360757	-0.225167
25	1	3.362066	-2.735610	0.642823
26	1	2.237472	-3.225829	-0.608710
27	1	3.481509	-2.037402	-1.023508
28	1	-0.986080	-2.249147	-0.006049
29	6	-3.170965	0.373787	0.590805
30	1	-3.715117	1.095591	-0.027165
31	1	-2.641276	0.938225	1.364545
32	1	-3.910830	-0.259154	1.092224
33	1	-1.969718	-1.894288	1.413387
34	6	-0.356989	2.930472	0.638694
35	1	-0.839534	3.234818	-0.294766
36	1	-1.139302	2.644845	1.347508
37	1	0.146453	3.811720	1.048056
38	1	1.240992	-0.587115	-1.744111
39	1	0.953582	-2.357229	1.850335
40	1	1.162482	1.641948	1.390842

TS(C'→F')

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -586.056748 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.363225 H
mPW1PW91/6-31+G(d,p): Electronic Energy: -586.252406 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.896962	-0.395785	-0.810067
2	1	-4.474109	0.528742	-0.919476
3	1	-3.646502	-0.760329	-1.812278
4	1	-4.549940	-1.136737	-0.337887
5	6	-2.636840	-0.168208	0.035741
6	6	-1.770660	-1.446962	0.169645
7	6	-0.283449	-1.004371	0.293616
8	6	0.641205	-1.818905	-0.689543
9	1	0.453712	-2.880154	-0.492307
10	6	2.058632	-1.391050	-0.419453
11	6	2.447603	-0.231008	-0.978593
12	6	3.147023	0.847758	-0.192848
13	1	4.033391	0.518241	0.355071
14	1	3.446699	1.695336	-0.815347
15	6	2.060765	1.273631	0.859404
16	6	0.706888	1.502958	0.181523
17	6	-1.651504	0.807008	-0.659898
18	1	-1.548539	0.543657	-1.723083
19	1	-1.975098	1.847738	-0.611027
20	6	2.779481	-2.089123	0.704761
21	1	2.985505	-3.125202	0.408124
22	1	3.737909	-1.625731	0.947467
23	1	2.181874	-2.150605	1.624134
24	1	-2.079603	-2.065527	1.017059
25	6	-3.031813	0.376599	1.422884
26	1	-3.551461	1.337251	1.339837
27	1	-2.168667	0.517524	2.088179
28	1	-3.704154	-0.322631	1.929191
29	1	1.879111	0.127058	-1.838722
30	1	0.338845	-1.615188	-1.723182
31	6	-0.309140	0.521318	-0.005956
32	1	-0.288362	1.197156	1.080627
33	6	0.534485	2.905882	-0.344476
34	1	-0.421563	3.105627	-0.821431
35	1	0.720971	3.643852	0.441011
36	1	1.321884	3.049611	-1.095709
37	1	2.346731	2.191510	1.384631
38	1	1.980999	0.470403	1.596074
39	1	-1.885031	-2.060531	-0.730560
40	1	0.091106	-1.169523	1.309168

SI-1: Cation C Bn Analog (Reactant; X=H)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -817.073861 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.448078 H
M06-2X/6-31+G(d,p): Electronic Energy: -817.0852731 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.276594	0.179457	-0.968797
2	1	-0.522143	-0.562183	-0.908406
3	6	1.352587	-0.421976	-1.992442
4	1	2.045222	0.389821	-2.235988
5	1	0.854464	-0.786184	-2.892168
6	6	2.017504	-1.456661	-1.213047
7	6	1.694231	-2.882627	-1.381806
8	1	1.586069	-3.150331	-2.437591
9	1	2.392094	-3.545221	-0.866782
10	1	0.696062	-3.039867	-0.931980
11	6	2.869890	-0.969965	-0.137559
12	1	3.859213	-0.797581	-0.598309
13	6	3.001368	-1.672316	1.241919
14	1	3.924676	-2.225932	1.420330
15	1	2.152523	-2.321845	1.471581
16	6	2.890737	-0.267074	1.901001
17	1	3.868430	0.122854	2.196557
18	1	2.207629	-0.189281	2.750686
19	6	2.391269	0.378634	0.567050
20	6	0.834103	0.426255	0.467784
21	1	0.472387	-0.398380	1.093838
22	6	3.125169	1.655921	0.155455
23	1	2.772225	2.068399	-0.795440
24	1	3.000680	2.433812	0.914200
25	1	4.200605	1.472308	0.064993
26	6	0.151883	1.744079	0.933124
27	1	-0.322862	1.622794	1.910698
28	1	0.892085	2.539419	1.050355
29	6	-0.879839	2.176937	-0.156885
30	6	-2.342749	1.728932	0.175745
31	1	-2.616675	2.223407	1.115673
32	1	-2.993284	2.157600	-0.595499
33	6	-0.320656	1.512330	-1.447070
34	1	-1.081518	1.376715	-2.222291
35	6	-0.906523	3.709551	-0.308990
36	1	-1.251715	4.188099	0.613981
37	1	0.089875	4.103172	-0.537129
38	1	-1.582406	4.017915	-1.113764
39	1	0.465361	2.151751	-1.867845
40	6	-2.654386	0.249592	0.292325
41	6	-2.464010	-0.447297	1.497560
42	6	-3.178007	-0.460172	-0.801921
43	6	-2.750039	-1.812057	1.596495
44	1	-2.116177	0.087521	2.377829
45	6	-3.467320	-1.824565	-0.709341
46	1	-3.382734	0.066168	-1.731240
47	6	-3.245528	-2.508648	0.489804
48	1	-2.611687	-2.324707	2.544274
49	1	-3.887807	-2.346277	-1.564338
50	1	-3.488254	-3.563942	0.571349

TS(C→F) Bn Analog (X=H)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -817.029846 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.44495 H
M06-2X/6-31+G(d,p): Electronic Energy: -817.0400644 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.441600	-0.995380	-0.885386
2	1	-0.315219	0.014575	-1.285215
3	6	-1.745569	-1.571535	-1.526219
4	1	-2.036522	-2.503832	-1.030053
5	1	-1.509177	-1.806286	-2.570448
6	6	-2.767620	-0.485489	-1.358245
7	6	-2.770521	0.630555	-2.369323
8	1	-3.176945	0.251004	-3.315328
9	1	-3.396177	1.472612	-2.066299
10	1	-1.765146	1.009178	-2.595471
11	6	-3.352913	-0.443073	-0.153013
12	1	-3.354006	-1.365075	0.432765
13	6	-3.466829	0.799835	0.663413
14	1	-4.433705	0.963276	1.154419
15	1	-3.245138	1.691418	0.072438
16	6	-2.422993	0.608972	1.792332
17	1	-2.927356	0.052986	2.595474
18	1	-2.158426	1.568127	2.258320
19	6	-1.107328	-0.197746	1.704584
20	6	-0.344482	-0.843880	0.678844
21	1	-0.092892	0.388360	0.952471
22	6	-0.559004	-0.333125	3.127602
23	1	-0.609674	-1.381522	3.441254
24	1	0.481068	-0.013444	3.212469
25	1	-1.145015	0.261590	3.827294
26	6	0.874669	-1.674471	1.097386
27	1	1.386103	-1.322576	1.991815
28	1	0.470336	-2.669681	1.341451
29	6	1.813949	-1.791902	-0.121399
30	6	2.814358	-0.593141	-0.218195
31	1	3.415132	-0.752188	-1.120778
32	1	3.506236	-0.678167	0.628698
33	6	0.796449	-1.839468	-1.278016
34	1	1.216026	-1.496554	-2.228531
35	6	2.648121	-3.082525	-0.047075
36	1	3.319447	-3.076685	0.818408
37	1	2.005338	-3.966016	0.029243
38	1	3.266522	-3.197402	-0.943152
39	1	0.480337	-2.878591	-1.430193
40	6	2.255383	0.816467	-0.244142
41	6	2.049300	1.534472	0.949353
42	6	1.962453	1.463101	-1.456651
43	6	1.531994	2.835814	0.934452
44	1	2.354273	1.093873	1.896499
45	6	1.448920	2.762542	-1.477558
46	1	2.159047	0.951977	-2.395774
47	6	1.219765	3.449959	-0.281380
48	1	1.406494	3.378475	1.867160
49	1	1.244820	3.245751	-2.428460
50	1	0.835203	4.464926	-0.298675

SI-4: Cation F Bn Analog (Product; X=H)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -817.097558 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.44799 H
M06-2X/6-31+G(d,p): Electronic Energy: -817.1094136 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.319424	-2.558562	-1.954239
2	1	0.028066	-2.406737	-2.998982
3	1	1.415851	-2.546105	-1.913031
4	1	-0.010327	-3.560803	-1.659099
5	6	-0.295800	-1.478328	-1.041302
6	6	0.140796	-1.720554	0.437962
7	6	0.605236	-0.368995	1.022393
8	1	-0.214110	0.148228	1.528870
9	6	1.838661	-0.533059	1.934967
10	1	2.025889	0.382304	2.532635
11	6	2.976350	-0.610112	0.999311
12	6	2.645498	0.014080	-0.276255
13	6	3.524109	1.348657	-0.451471
14	1	4.016823	1.626276	0.486578
15	1	4.301224	1.194208	-1.201876
16	6	2.459386	2.387739	-0.820948
17	1	2.240834	2.341632	-1.894521
18	1	2.800786	3.402566	-0.593247
19	6	1.215174	1.981851	-0.012113
20	6	1.132584	0.431632	-0.206143
21	6	0.269990	-0.059773	-1.391624
22	1	0.830674	-0.072488	-2.333206
23	1	-0.555959	0.638239	-1.534005
24	6	4.255168	-1.255059	1.312885
25	1	4.529554	-1.147290	2.367504
26	1	4.079819	-2.337356	1.165584
27	1	5.070384	-0.961024	0.649393
28	1	0.977863	-2.434250	0.447973
29	6	-1.847962	-1.553618	-1.228200
30	1	-2.057735	-1.356294	-2.286318
31	1	-2.146021	-2.593763	-1.047755
32	1	-0.645786	-2.175414	1.044092
33	6	-0.034301	2.804069	-0.330631
34	1	-0.253719	2.812977	-1.402766
35	1	-0.917420	2.424741	0.191607
36	1	0.114640	3.842737	-0.019313
37	1	2.912369	-0.655214	-1.106028
38	1	1.821528	-1.349235	2.666751
39	1	1.455296	2.159259	1.049106
40	6	-2.714134	-0.643087	-0.379662
41	6	-3.152203	0.599355	-0.866788
42	6	-3.147164	-1.034742	0.898997
43	6	-3.960985	1.437214	-0.093749
44	1	-2.883408	0.904902	-1.875285
45	6	-3.952983	-0.200469	1.678296
46	1	-2.883884	-2.018776	1.279285
47	6	-4.356621	1.044082	1.187116
48	1	-4.296283	2.387180	-0.499866
49	1	-4.284207	-0.532563	2.657983
50	1	-4.994081	1.688129	1.785117

SI-2: Cation C Bn Analog (Reactant; X=NMe_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -950.987672 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.520748 H
M06-2X/6-31+G(d,p): Electronic Energy: -951.0018966 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.160262	0.235141	0.976002
2	1	-0.074993	0.121688	0.984317
3	6	-1.716264	-0.828971	2.039599
4	1	-2.772785	-0.592207	2.197825
5	1	-1.159744	-0.749402	2.974699
6	6	-1.560043	-2.103260	1.353915
7	6	-0.427681	-2.999233	1.642741
8	1	-0.237871	-3.078060	2.717901
9	1	-0.529951	-3.983252	1.181692
10	1	0.476036	-2.524416	1.214614
11	6	-2.461870	-2.317374	0.226016
12	1	-3.377361	-2.771872	0.644037
13	6	-2.030834	-3.025701	-1.088371
14	1	-2.391531	-4.045295	-1.234918
15	1	-0.948676	-3.010141	-1.242749
16	6	-2.770960	-1.901882	-1.868634
17	1	-3.759006	-2.224355	-2.208383
18	1	-2.231211	-1.467982	-2.714382
19	6	-2.863877	-1.007753	-0.589269
20	6	-1.675621	-0.000196	-0.478659
21	1	-0.848541	-0.457526	-1.034464
22	6	-4.253942	-0.435798	-0.305549
23	1	-4.296629	0.158466	0.613193
24	1	-4.582345	0.208560	-1.126316
25	1	-4.991981	-1.240050	-0.220314
26	6	-1.924737	1.427794	-1.041462
27	1	-1.452498	1.563691	-2.018849
28	1	-2.993473	1.599029	-1.191987
29	6	-1.399669	2.464760	0.001429
30	6	0.060420	2.942672	-0.296787
31	1	0.038209	3.422149	-1.283801
32	1	0.289666	3.738986	0.421666
33	6	-1.508440	1.685516	1.342767
34	1	-0.853813	2.087166	2.122816
35	6	-2.293849	3.717907	0.025334
36	1	-2.255555	4.244746	-0.934475
37	1	-3.339418	3.456432	0.221522
38	1	-1.971476	4.420951	0.800996
39	1	-2.539036	1.749666	1.714021
40	6	1.190462	1.935047	-0.265471
41	6	1.525928	1.149597	-1.380633
42	6	1.995222	1.775398	0.875068
43	6	2.570319	0.228276	-1.356004
44	1	0.976845	1.276567	-2.310763
45	6	3.045278	0.861838	0.926594
46	1	1.812873	2.398534	1.747983
47	6	3.362123	0.048952	-0.192071
48	1	2.794555	-0.322706	-2.260994
49	1	3.641479	0.810425	1.829079
50	7	4.402043	-0.862350	-0.155740
51	6	4.837783	-1.507488	-1.388902
52	6	5.323393	-0.857187	0.974643
53	1	5.646448	-2.201870	-1.160335
54	1	4.023930	-2.085922	-1.840204
55	1	5.202753	-0.785991	-2.134671
56	1	4.793166	-1.041239	1.915481
57	1	6.050072	-1.659371	0.844991
58	1	5.870289	0.092729	1.067173

TS(C→F) Bn Analog (X=NMe_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -950.945324 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.518006 H
M06-2X/6-31+G(d,p): Electronic Energy: -950.9602162 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.835417	0.304797	-0.835342
2	1	-0.846176	0.421869	-1.284957
3	6	-2.689676	1.531509	-1.299281
4	1	-3.610035	1.605072	-0.709492
5	1	-2.973161	1.349340	-2.342113
6	6	-1.782613	2.713136	-1.109980
7	6	-0.793471	3.007386	-2.206722
8	1	-1.333756	3.407488	-3.073990
9	1	-0.053316	3.755469	-1.915813
10	1	-0.263675	2.112392	-2.558657
11	6	-1.708575	3.177492	0.145749
12	1	-2.550579	2.960938	0.807064
13	6	-0.418668	3.419971	0.856494
14	1	-0.360923	4.349168	1.436251
15	1	0.426722	3.414170	0.164801
16	6	-0.311967	2.253813	1.874943
17	1	-0.804653	2.599842	2.793336
18	1	0.729943	2.081870	2.176891
19	6	-0.954908	0.851763	1.738245
20	6	-1.588290	0.099183	0.700998
21	1	-0.309020	-0.028803	0.896454
22	6	-0.919882	0.195655	3.120806
23	1	-1.932805	0.180222	3.539038
24	1	-0.554219	-0.830936	3.096091
25	1	-0.280452	0.759155	3.799945
26	6	-2.252403	-1.235681	1.045476
27	1	-1.846979	-1.747505	1.916280
28	1	-3.294811	-0.975705	1.289818
29	6	-2.228122	-2.102397	-0.229573
30	6	-0.875249	-2.870279	-0.382793
31	1	-0.923571	-3.413362	-1.334335
32	1	-0.846917	-3.636697	0.401737
33	6	-2.453908	-1.032561	-1.318182
34	1	-2.048254	-1.324440	-2.291460
35	6	-3.361148	-3.142015	-0.215127
36	1	-3.240720	-3.855593	0.607345
37	1	-4.340090	-2.662631	-0.106425
38	1	-3.373325	-3.715017	-1.148132
39	1	-3.532432	-0.891290	-1.456930
40	6	0.416793	-2.079077	-0.328951
41	6	1.148708	-1.942008	0.863991
42	6	0.990642	-1.505697	-1.478081
43	6	2.349790	-1.233968	0.930770
44	1	0.798883	-2.444587	1.764127
45	6	2.188315	-0.799884	-1.440723
46	1	0.500859	-1.635586	-2.440527
47	6	2.905782	-0.628382	-0.226109
48	1	2.878059	-1.200315	1.875479
49	1	2.585944	-0.409782	-2.369061
50	7	4.090229	0.074333	-0.179371
51	6	4.904096	0.039229	1.031089
52	6	4.721125	0.512262	-1.420691
53	1	5.780817	0.670646	0.888443
54	1	4.350829	0.433851	1.890656
55	1	5.246902	-0.976462	1.276224
56	1	4.054338	1.169133	-1.989557
57	1	5.617945	1.083262	-1.181050
58	1	5.011291	-0.330992	-2.063929

SI-5: Cation F Bn Analog (Product; X=NMe_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -951.013861 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.520288 H
M06-2X/6-31+G(d,p): Electronic Energy: -951.0241787 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.003735	2.867704	-1.376639
2	1	-1.905827	2.978996	-2.461872
3	1	-3.046360	2.597890	-1.166804
4	1	-1.818746	3.847787	-0.922991
5	6	-1.024855	1.806889	-0.834526
6	6	-1.183172	1.670500	0.713480
7	6	-1.326432	0.169168	1.047450
8	1	-0.359479	-0.268505	1.311467
9	6	-2.390764	-0.085278	2.136471
10	1	-2.287163	-1.101271	2.567192
11	6	-3.674009	-0.090203	1.406497
12	6	-3.471749	-0.372447	-0.018590
13	6	-4.126239	-1.765715	-0.441019
14	1	-4.459033	-2.324188	0.440400
15	1	-4.997909	-1.607170	-1.078692
16	6	-2.962367	-2.494705	-1.127182
17	1	-2.900046	-2.203646	-2.182830
18	1	-3.090774	-3.581194	-1.091294
19	6	-1.705530	-2.017747	-0.378452
20	6	-1.919905	-0.476611	-0.239593
21	6	-1.375341	0.389689	-1.398426
22	1	-2.083309	0.456045	-2.232607
23	1	-0.474410	-0.079192	-1.795985
24	6	-4.975245	0.192651	2.026987
25	1	-5.027554	-0.158884	3.062937
26	1	-5.065100	1.293422	2.083071
27	1	-5.822359	-0.172148	1.442022
28	1	-2.086303	2.209796	1.031842
29	6	0.418103	2.261054	-1.241439
30	1	0.451055	2.297448	-2.337564
31	1	0.537183	3.296915	-0.899593
32	1	-0.353881	2.124007	1.261242
33	6	-0.388501	-2.498366	-0.989751
34	1	-0.322298	-2.257978	-2.055411
35	1	0.479556	-2.056882	-0.490640
36	1	-0.308636	-3.586139	-0.895376
37	1	-3.961342	0.414780	-0.612070
38	1	-2.386034	0.589921	3.001194
39	1	-1.762699	-2.439930	0.638381
40	6	1.592859	1.447628	-0.741678
41	6	2.154713	0.412229	-1.507865
42	6	2.226185	1.733856	0.481343
43	6	3.250986	-0.325872	-1.074132
44	1	1.744567	0.190672	-2.490337
45	6	3.321771	1.010708	0.940458
46	1	1.877673	2.570231	1.082547
47	6	3.862826	-0.056326	0.177659
48	1	3.647062	-1.096533	-1.723444
49	1	3.774964	1.295997	1.881485
50	7	4.943185	-0.787073	0.623781
51	6	5.547711	-1.797073	-0.235322
52	6	5.625083	-0.407436	1.854482
53	1	6.358279	-2.286293	0.304218
54	1	4.818968	-2.567252	-0.514269
55	1	5.961688	-1.363097	-1.156410
56	1	4.937619	-0.420383	2.708533
57	1	6.421022	-1.123577	2.057192
58	1	6.072976	0.594085	1.786727

SI-3: Cation C Bn Analog (Reactant; X=NO_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1021.580515 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.450079 H
M06-2X/6-31+G(d,p): Electronic Energy: -1021.5120669 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.063558	0.226583	0.991310
2	1	0.015007	0.057813	1.026173
3	6	-1.697102	-0.827248	2.003994
4	1	-2.747445	-0.542148	2.136851
5	1	-1.177243	-0.803326	2.963366
6	6	-1.619295	-2.114810	1.319025
7	6	-0.672325	-3.161052	1.732020
8	1	-0.677193	-3.291205	2.820397
9	1	-0.816458	-4.109551	1.212855
10	1	0.342910	-2.793431	1.494110
11	6	-2.439608	-2.232731	0.122882
12	1	-3.383061	-2.691713	0.475741
13	6	-1.957984	-2.932767	-1.185661
14	1	-2.338072	-3.938588	-1.369966
15	1	-0.869187	-2.943369	-1.281772
16	6	-2.632589	-1.770196	-1.968908
17	1	-3.612656	-2.058896	-2.358070
18	1	-2.043651	-1.334732	-2.780065
19	6	-2.758476	-0.902786	-0.672081
20	6	-1.541431	0.060351	-0.486362
21	1	-0.713539	-0.407824	-1.032055
22	6	-4.140257	-0.288307	-0.438030
23	1	-4.206390	0.281332	0.495170
24	1	-4.408714	0.388961	-1.253637
25	1	-4.908865	-1.067437	-0.409999
26	6	-1.725249	1.512997	-1.010198
27	1	-1.227633	1.659765	-1.973078
28	1	-2.782836	1.726944	-1.180550
29	6	-1.193977	2.501673	0.074980
30	6	0.277505	2.973788	-0.188901
31	1	0.271804	3.504344	-1.148372
32	1	0.518778	3.721655	0.574900
33	6	-1.349245	1.684905	1.388996
34	1	-0.693938	2.037174	2.192119
35	6	-2.059280	3.775711	0.126329
36	1	-1.993739	4.332529	-0.814622
37	1	-3.112783	3.530196	0.296844
38	1	-1.735667	4.444824	0.930639
39	1	-2.381616	1.782122	1.747277
40	6	1.383962	1.941262	-0.211694
41	6	1.692114	1.226720	-1.383328
42	6	2.150114	1.686844	0.940404
43	6	2.685161	0.248719	-1.396844
44	1	1.161237	1.448628	-2.304448
45	6	3.148789	0.714315	0.949426
46	1	1.971307	2.266235	1.841989
47	6	3.386164	-0.008613	-0.219146
48	1	2.928702	-0.302613	-2.297249
49	1	3.742903	0.516710	1.833714
50	7	4.410370	-1.071082	-0.211386
51	8	5.001810	-1.283574	0.847058
52	8	4.593796	-1.692549	-1.258038

TS(C→F) Bn Analog (X=NO_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1021.531237 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.447522 H
M06-2X/6-31+G(d,p): Electronic Energy: -1021.4636315 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.594228	0.155075	-0.978464
2	1	-0.534336	0.201946	-1.246358
3	6	-2.303592	1.300418	-1.768412
4	1	-3.337398	1.416286	-1.425410
5	1	-2.331279	0.988382	-2.818845
6	6	-1.473011	2.523477	-1.513353
7	6	-0.237429	2.717197	-2.351838
8	1	-0.539504	2.998643	-3.368538
9	1	0.406996	3.514738	-1.976975
10	1	0.364760	1.804466	-2.452331
11	6	-1.735610	3.150732	-0.357994
12	1	-2.719843	2.985461	0.086402
13	6	-0.684640	3.552703	0.620448
14	1	-0.803415	4.546528	1.068220
15	1	0.315290	3.509819	0.182541
16	6	-0.830148	2.528535	1.772380
17	1	-1.611891	2.914574	2.443175
18	1	0.071129	2.506727	2.400205
19	6	-1.299143	1.061000	1.652892
20	6	-1.621464	0.142731	0.597043
21	1	-0.410672	0.209828	1.022633
22	6	-1.489693	0.526344	3.075922
23	1	-2.550327	0.316795	3.251337
24	1	-0.937654	-0.397495	3.259347
25	1	-1.158898	1.258046	3.811676
26	6	-2.199176	-1.223719	0.989140
27	1	-1.823351	-1.628826	1.927734
28	1	-3.274668	-1.041917	1.141800
29	6	-2.014438	-2.193559	-0.197076
30	6	-0.646910	-2.955340	-0.144499
31	1	-0.616364	-3.614247	-1.019022
32	1	-0.673518	-3.610965	0.734139
33	6	-2.141774	-1.232218	-1.393998
34	1	-1.634609	-1.597360	-2.292034
35	6	-3.124657	-3.259898	-0.205593
36	1	-3.075329	-3.898751	0.682808
37	1	-4.116367	-2.796403	-0.233652
38	1	-3.035731	-3.907946	-1.083311
39	1	-3.202021	-1.127907	-1.654012
40	6	0.632244	-2.145523	-0.101847
41	6	1.178734	-1.723713	1.126419
42	6	1.328525	-1.823472	-1.279660
43	6	2.348912	-0.964345	1.181244
44	1	0.713131	-2.039463	2.056961
45	6	2.502680	-1.071090	-1.246991
46	1	0.958684	-2.179868	-2.236806
47	6	2.983545	-0.632810	-0.014386
48	1	2.782808	-0.649629	2.123190
49	1	3.046564	-0.827222	-2.152065
50	7	4.210172	0.191252	0.030888
51	8	4.780107	0.416926	-1.033783
52	8	4.567924	0.609555	1.131624

SI-6: Cation F Bn Analog (Product; X=NO_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1021.603665 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.450159 H
M06-2X/6-31+G(d,p): Electronic Energy: -1021.536508 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.874900	2.953018	-1.250522
2	1	-1.741356	3.118150	-2.324726
3	1	-2.922489	2.670568	-1.088906
4	1	-1.709147	3.909425	-0.742703
5	6	-0.910421	1.867989	-0.727848
6	6	-1.131066	1.655218	0.804353
7	6	-1.260632	0.137550	1.062680
8	1	-0.299858	-0.302341	1.343665
9	6	-2.361695	-0.180478	2.096123
10	1	-2.282250	-1.222190	2.468784
11	6	-3.615959	-0.156065	1.319961
12	6	-3.356990	-0.381729	-0.097214
13	6	-3.975072	-1.799588	-0.535311
14	1	-4.272539	-2.389239	0.338321
15	1	-4.861566	-1.650813	-1.153896
16	6	-2.789829	-2.461780	-1.247764
17	1	-2.736069	-2.124324	-2.289719
18	1	-2.891287	-3.551589	-1.255113
19	6	-1.548905	-1.985095	-0.473884
20	6	-1.798150	-0.453685	-0.275094
21	6	-1.233072	0.477258	-1.372871
22	1	-1.920168	0.580994	-2.220214
23	1	-0.319859	0.034347	-1.772151
24	6	-4.937748	0.090587	1.903439
25	1	-5.029198	-0.312054	2.917730
26	1	-5.005038	1.188962	2.018797
27	1	-5.765753	-0.223838	1.265644
28	1	-2.059845	2.162553	1.101495
29	6	0.538961	2.356494	-1.068234
30	1	0.594323	2.480353	-2.156051
31	1	0.653861	3.359413	-0.640022
32	1	-0.343051	2.102857	1.413941
33	6	-0.218119	-2.413418	-1.093339
34	1	-0.143157	-2.122108	-2.145520
35	1	0.636169	-1.984990	-0.560779
36	1	-0.119770	-3.502359	-1.048608
37	1	-3.864381	0.386290	-0.697956
38	1	-2.397602	0.437503	3.001233
39	1	-1.601265	-2.448446	0.524961
40	6	1.704090	1.498970	-0.618095
41	6	2.279467	0.553506	-1.485019
42	6	2.269857	1.652511	0.660666
43	6	3.348403	-0.246598	-1.084058
44	1	1.903317	0.454860	-2.499434
45	6	3.336285	0.861171	1.084098
46	1	1.894534	2.421713	1.329313
47	6	3.851224	-0.090677	0.205898
48	1	3.797333	-0.972558	-1.751246
49	1	3.777721	0.979851	2.066284
50	7	4.969717	-0.946222	0.649683
51	8	5.401926	-1.776518	-0.148991
52	8	5.391322	-0.782032	1.794155

SI-7: Cation C' Bn Analog (Reactant; X=H)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -817.074112 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.448238 H
M06-2X/6-31+G(d,p): Electronic Energy: -817.0856883 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.830206	3.433174	0.960168
2	1	-1.212949	3.503211	1.984046
3	1	0.210574	3.777556	0.970398
4	1	-1.405200	4.131648	0.342824
5	6	-0.941935	1.992909	0.423849
6	6	-0.293250	1.873864	-0.999601
7	6	0.822210	0.806214	-0.905749
8	6	2.256286	1.533494	-0.683313
9	1	2.420362	2.276057	-1.464193
10	6	3.152269	0.397618	-0.750839
11	6	3.146968	-0.520513	0.379310
12	6	3.435013	-2.020538	0.141698
13	1	3.988326	-2.296382	-0.757618
14	1	3.937031	-2.473124	0.998234
15	6	1.903866	-2.277075	0.136889
16	6	1.635662	-0.923380	0.867933
17	6	-0.114361	1.013999	1.306126
18	1	0.677358	1.570353	1.825282
19	1	-0.721825	0.549844	2.086445
20	6	3.882247	0.091841	-2.001302
21	1	4.909755	-0.213912	-1.763907
22	1	3.433236	-0.787772	-2.486472
23	1	3.888108	0.923120	-2.706538
24	1	-1.020605	1.539548	-1.743520
25	6	-2.464992	1.627688	0.393134
26	1	-2.862357	1.825077	1.395917
27	1	-2.955944	2.344231	-0.276558
28	1	3.683655	-0.016967	1.199929
29	1	2.210215	2.000842	0.303095
30	6	0.493273	-0.031137	0.344403
31	1	-0.316690	-0.715678	0.055663
32	6	1.595934	-1.132725	2.384234
33	1	1.689822	-0.195045	2.937876
34	1	0.642678	-1.595305	2.661296
35	1	2.392467	-1.804019	2.717885
36	1	1.547292	-3.171078	0.654902
37	1	1.498759	-2.275337	-0.881040
38	1	0.089576	2.836947	-1.350641
39	1	0.878417	0.210316	-1.822149
40	6	-2.858268	0.221497	-0.017163
41	6	-2.998476	-0.797414	0.940998
42	6	-3.131708	-0.097072	-1.358096
43	6	-3.359421	-2.095301	0.569988
44	1	-2.851730	-0.567747	1.993723
45	6	-3.493185	-1.393729	-1.735472
46	1	-3.097484	0.683587	-2.114279
47	6	-3.599589	-2.400637	-0.772805
48	1	-3.475471	-2.861316	1.331351
49	1	-3.713255	-1.610324	-2.776803
50	1	-3.894146	-3.404988	-1.061487

SI-8: TS(C'→F') Bn Analog (X=H)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -817.050043 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.444959 H
M06-2X/6-31+G(d,p): Electronic Energy: -817.0635953 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.765223	3.537604	0.611935
2	1	-2.388106	3.543274	1.512924
3	1	-0.895779	4.177143	0.797834
4	1	-2.348006	3.993725	-0.194907
5	6	-1.334121	2.110148	0.235597
6	6	-0.375338	2.106800	-0.987540
7	6	0.711055	1.016914	-0.767096
8	6	2.163523	1.613642	-0.922540
9	1	2.193218	2.130092	-1.888425
10	6	3.122097	0.456806	-0.823561
11	6	3.401099	0.018304	0.417022
12	6	3.326811	-1.438678	0.793689
13	1	3.901297	-2.109670	0.149883
14	1	3.648106	-1.622829	1.822833
15	6	1.803713	-1.772485	0.605419
16	6	0.919973	-0.711540	1.270855
17	6	-0.453598	1.485668	1.349902
18	1	0.220085	2.251725	1.761694
19	1	-1.033804	1.088845	2.184133
20	6	3.384847	-0.317323	-2.089461
21	1	3.974814	0.305046	-2.774051
22	1	3.951383	-1.234523	-1.915934
23	1	2.464526	-0.575740	-2.630146
24	1	-0.911586	1.955597	-1.927688
25	6	-2.633182	1.274003	-0.012219
26	1	-3.271519	1.389267	0.871610
27	1	-3.167171	1.753631	-0.840583
28	1	3.226961	0.709597	1.243094
29	1	2.336507	2.362380	-0.140700
30	6	0.430862	0.465279	0.651490
31	1	-0.269527	-0.635066	0.600567
32	6	0.652353	-0.994133	2.729603
33	1	0.072504	-0.233017	3.246068
34	1	0.171003	-1.969241	2.850057
35	1	1.630011	-1.066159	3.221187
36	1	1.550800	-2.750025	1.030371
37	1	1.600846	-1.808296	-0.467394
38	1	0.113075	3.083925	-1.064434
39	1	0.606038	0.207198	-1.494953
40	6	-2.489310	-0.207334	-0.310164
41	6	-2.623761	-1.161841	0.716550
42	6	-2.261792	-0.676871	-1.616638
43	6	-2.503559	-2.531564	0.454327
44	1	-2.866719	-0.831523	1.724044
45	6	-2.141158	-2.043464	-1.882921
46	1	-2.208943	0.030515	-2.439896
47	6	-2.252739	-2.976165	-0.846967
48	1	-2.636468	-3.248962	1.259055
49	1	-1.982609	-2.381069	-2.902873
50	1	-2.176256	-4.038455	-1.057050

SI-9: Cation F' Bn Analog (Product; X=H)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -817.095346 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.448763 H
M06-2X/6-31+G(d,p): Electronic Energy: -817.1123216 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.082551	3.438930	-1.150251
2	1	0.335469	3.547101	-2.156800
3	1	-1.166461	3.585315	-1.222043
4	1	0.324323	4.249091	-0.535496
5	6	0.255987	2.059242	-0.550202
6	6	-0.418230	1.893703	0.834549
7	6	-0.759848	0.400430	1.020433
8	6	-2.121058	0.210137	1.730615
9	1	-2.163243	-0.706918	2.345414
10	6	-3.110250	0.045022	0.640117
11	6	-2.465525	-0.442493	-0.546306
12	6	-2.665462	-2.052000	-0.236018
13	1	-3.427404	-2.285941	0.514543
14	1	-3.024733	-2.457800	-1.184219
15	6	-1.262487	-2.525065	0.152649
16	6	-0.287419	-1.610212	-0.608784
17	6	-0.393111	0.920489	-1.394500
18	1	-1.225597	1.339218	-1.972823
19	1	0.308678	0.522817	-2.129843
20	6	-4.543100	0.352707	0.772595
21	1	-4.621266	1.446220	0.635619
22	1	-5.159640	-0.114651	0.002122
23	1	-4.927492	0.145698	1.775814
24	1	0.193285	2.282544	1.655046
25	6	1.818001	1.978920	-0.488563
26	1	2.185594	2.178394	-1.501879
27	1	2.151124	2.824850	0.125585
28	1	-2.964986	-0.212323	-1.488916
29	1	-2.409701	1.015829	2.417096
30	6	-0.921357	-0.191692	-0.440981
31	1	0.701137	-1.628023	-0.142468
32	6	-0.138008	-2.066006	-2.070708
33	1	0.611259	-1.480424	-2.607012
34	1	0.188944	-3.110020	-2.102364
35	1	-1.075851	-1.995598	-2.634802
36	1	-1.142855	-3.583725	-0.102270
37	1	-1.111655	-2.449120	1.235222
38	1	-1.345931	2.484101	0.839648
39	1	0.038658	-0.114079	1.558506
40	6	2.492650	0.720150	0.019689
41	6	3.015947	-0.222879	-0.879216
42	6	2.680327	0.492192	1.393873
43	6	3.673426	-1.370314	-0.425785
44	1	2.932312	-0.044798	-1.948747
45	6	3.331432	-0.655028	1.854353
46	1	2.340901	1.234084	2.112888
47	6	3.825621	-1.595255	0.944700
48	1	4.082133	-2.076784	-1.142479
49	1	3.475777	-0.802372	2.920856
50	1	4.347312	-2.478554	1.300244

SI-10: Cation C' Bn Analog (Reactant; X=NMe_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -950.994996 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.52105 H
M06-2X/6-31+G(d,p): Electronic Energy: -951.0070192 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.076315	3.493314	0.431379
2	1	1.945447	3.824200	1.467736
3	1	3.128635	3.217178	0.298129
4	1	1.875090	4.352052	-0.218071
5	6	1.140366	2.318741	0.099102
6	6	1.401094	1.767014	-1.350613
7	6	1.775939	0.270923	-1.226192
8	6	3.329445	0.048514	-1.209685
9	1	3.638426	-0.199986	-2.234483
10	6	3.846222	-1.011267	-0.268973
11	6	3.359148	-2.285843	-0.241330
12	6	2.276269	-2.860394	-1.137201
13	1	2.235011	-2.345540	-2.099094
14	1	2.451950	-3.919484	-1.339216
15	6	0.987031	-2.637587	-0.315862
16	6	1.355649	-1.493391	0.625650
17	6	1.422872	1.100496	1.029159
18	1	2.469659	1.108631	1.355611
19	1	0.804105	1.117298	1.930400
20	6	4.963343	-0.610859	0.656674
21	1	5.240487	-1.409351	1.348700
22	1	5.851128	-0.357260	0.062092
23	1	4.712519	0.288339	1.230320
24	1	0.506412	1.872422	-1.968119
25	6	-0.334729	2.820109	0.257302
26	1	-0.408837	3.313281	1.234321
27	1	-0.491731	3.605620	-0.492115
28	1	3.794496	-2.972435	0.483448
29	1	3.824655	0.992415	-0.967852
30	6	1.145435	-0.118054	0.139097
31	1	0.046172	-0.131300	-0.043585
32	6	1.412759	-1.762789	2.086105
33	1	2.017648	-1.035139	2.630392
34	1	0.377000	-1.659399	2.454651
35	1	1.734150	-2.780265	2.315495
36	1	0.731273	-3.526295	0.267327
37	1	0.120665	-2.374326	-0.931857
38	1	2.193752	2.327688	-1.856141
39	1	1.337700	-0.307770	-2.042839
40	6	-1.448906	1.795975	0.149660
41	6	-1.978542	1.166666	1.290801
42	6	-2.064565	1.478466	-1.074700
43	6	-3.020793	0.245533	1.221649
44	1	-1.591100	1.428456	2.273301
45	6	-3.108650	0.562300	-1.170143
46	1	-1.748706	1.986567	-1.982641
47	6	-3.613807	-0.097289	-0.020738
48	1	-3.399711	-0.175801	2.144520
49	1	-3.552656	0.387332	-2.141967
50	7	-4.640710	-1.017834	-0.105348
51	6	-5.279130	-1.498002	1.114581
52	6	-5.363814	-1.174756	-1.362289
53	1	-6.039768	-2.233271	0.851620
54	1	-4.554187	-1.994618	1.768863
55	1	-5.762320	-0.690019	1.683873
56	1	-4.686917	-1.473977	-2.169710
57	1	-6.107379	-1.963760	-1.248475
58	1	-5.881809	-0.253570	-1.667809

SI-11: TS(C'→F') Bn Analog (X=NMe_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -950.966178 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.517694 H
M06-2X/6-31+G(d,p): Electronic Energy: -950.9840136 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.732476	3.629026	0.105943
2	1	2.485552	4.226071	0.990583
3	1	3.769936	3.291498	0.204417
4	1	2.679561	4.292415	-0.763738
5	6	1.771384	2.440503	-0.055310
6	6	2.175639	1.538273	-1.254357
7	6	1.899315	0.056719	-0.872457
8	6	3.176034	-0.844875	-1.083521
9	1	3.523506	-0.672165	-2.108287
10	6	2.749741	-2.264907	-0.818074
11	6	2.660518	-2.629701	0.473593
12	6	1.444849	-3.319081	1.036462
13	1	1.137330	-4.218892	0.497325
14	1	1.570467	-3.597843	2.086644
15	6	0.315695	-2.240722	0.865889
16	6	0.774676	-0.869372	1.374459
17	6	1.882072	1.462801	1.142528
18	1	2.937189	1.350013	1.433112
19	1	1.339715	1.801958	2.025810
20	6	2.120438	-3.010850	-1.966601
21	1	2.892335	-3.239163	-2.712451
22	1	1.673649	-3.959492	-1.661563
23	1	1.356321	-2.420649	-2.490041
24	1	1.655106	1.821756	-2.173043
25	6	0.321126	3.006742	-0.192425
26	1	0.161831	3.702303	0.640479
27	1	0.300671	3.616275	-1.103982
28	1	3.222616	-2.039149	1.198705
29	1	3.971889	-0.518337	-0.404070
30	6	1.437835	0.114708	0.603120
31	1	0.122243	0.112077	0.693377
32	6	0.554564	-0.680821	2.857364
33	1	0.847890	0.292514	3.243389
34	1	-0.487758	-0.878396	3.120633
35	1	1.161353	-1.439639	3.366930
36	1	-0.594424	-2.523267	1.405769
37	1	0.070085	-2.181496	-0.196774
38	1	3.245637	1.660902	-1.453093
39	1	1.095165	-0.361985	-1.484159
40	6	-0.835298	2.024876	-0.220208
41	6	-1.591512	1.754351	0.935344
42	6	-1.265840	1.397539	-1.404739
43	6	-2.677031	0.879042	0.932604
44	1	-1.347492	2.266692	1.863887
45	6	-2.348816	0.524561	-1.435194
46	1	-0.761386	1.619248	-2.342098
47	6	-3.089009	0.227013	-0.259655
48	1	-3.232599	0.742512	1.852001
49	1	-2.642187	0.100467	-2.387231
50	7	-4.160091	-0.638722	-0.278071
51	6	-5.020297	-0.748715	0.895801
52	6	-4.665588	-1.138714	-1.553011
53	1	-5.794592	-1.490437	0.701040
54	1	-4.453711	-1.086469	1.770779
55	1	-5.510151	0.203253	1.145816
56	1	-3.888632	-1.687410	-2.096256
57	1	-5.484574	-1.832079	-1.362678
58	1	-5.039724	-0.332417	-2.200075

SI-12: Cation F' Bn Analog (Product; X=NMe_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -951.010092 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.521105 H
M06-2X/6-31+G(d,p): Electronic Energy: -951.027759 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.262556	3.442415	0.613135
2	1	2.073976	3.820335	1.623823
3	1	3.326514	3.187778	0.545813
4	1	2.070025	4.262680	-0.086985
5	6	1.374338	2.221880	0.300237
6	6	1.704217	1.653633	-1.102319
7	6	1.466433	0.130174	-1.060204
8	6	2.540095	-0.633573	-1.873707
9	1	2.153349	-1.588023	-2.278000
10	6	3.583054	-0.988731	-0.890672
11	6	3.010940	-1.100446	0.433852
12	6	2.595907	-2.673478	0.489101
13	1	3.129301	-3.301011	-0.231828
14	1	2.889399	-3.013367	1.484898
15	6	1.078257	-2.661958	0.287242
16	6	0.593832	-1.350220	0.930844
17	6	1.716187	1.034695	1.250421
18	1	2.728123	1.179497	1.648194
19	1	1.055682	1.021646	2.119165
20	6	5.002400	-1.183012	-1.221100
21	1	5.452004	-0.173201	-1.240141
22	1	5.544012	-1.760256	-0.468314
23	1	5.148459	-1.596025	-2.223958
24	1	1.133561	2.138413	-1.901022
25	6	-0.109065	2.707520	0.422425
26	1	-0.221136	3.130853	1.427966
27	1	-0.216863	3.550433	-0.272540
28	1	3.718996	-0.900781	1.242496
29	1	2.945364	-0.101998	-2.743242
30	6	1.652190	-0.301524	0.453472
31	1	-0.393905	-1.074511	0.551370
32	6	0.493066	-1.497584	2.459438
33	1	0.054111	-0.613725	2.926270
34	1	-0.153321	-2.345249	2.708519
35	1	1.465662	-1.672401	2.934394
36	1	0.625543	-3.551206	0.738851
37	1	0.824908	-2.694141	-0.778770
38	1	2.763212	1.854345	-1.319790
39	1	0.461261	-0.113328	-1.409669
40	6	-1.248055	1.739604	0.185708
41	6	-1.940701	1.152119	1.255992
42	6	-1.737199	1.459585	-1.102412
43	6	-3.027203	0.302625	1.066744
44	1	-1.641870	1.384454	2.275767
45	6	-2.817446	0.610228	-1.320987
46	1	-1.283552	1.941886	-1.965442
47	6	-3.493454	-0.006957	-0.236528
48	1	-3.529131	-0.098468	1.938312
49	1	-3.157124	0.455599	-2.337460
50	7	-4.562389	-0.856370	-0.439461
51	6	-5.343417	-1.324639	0.698873
52	6	-5.116887	-1.020091	-1.777264
53	1	-6.119033	-2.002964	0.343674
54	1	-4.716632	-1.878713	1.406853
55	1	-5.828900	-0.499384	1.239769
56	1	-4.358231	-1.390460	-2.476100
57	1	-5.920092	-1.756050	-1.742270
58	1	-5.527231	-0.081660	-2.178115

SI-13: Cation C' Bn Analog (Reactant; X=NO_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1021.585641 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.45075 H
M06-2X/6-31+G(d,p): Electronic Energy: -1021.5202453 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.600003	3.478816	0.637512
2	1	1.451609	3.751647	1.688049
3	1	2.668308	3.272346	0.500876
4	1	1.355640	4.354863	0.027374
5	6	0.729472	2.266265	0.250355
6	6	1.031476	1.791874	-1.216199
7	6	1.707896	0.406354	-1.113261
8	6	3.243768	0.530011	-1.026119
9	1	3.692357	0.741525	-2.004573
10	6	3.979403	-0.555294	-0.333394
11	6	3.288075	-1.517060	0.448340
12	6	3.029494	-2.603170	-0.808596
13	1	3.168256	-2.204426	-1.815399
14	1	3.678693	-3.467344	-0.669594
15	6	1.566990	-2.669621	-0.330159
16	6	1.747952	-1.484444	0.677971
17	6	1.087493	1.027396	1.133959
18	1	2.079996	1.168071	1.585020
19	1	0.393464	0.893014	1.966245
20	6	5.459183	-0.624762	-0.464530
21	1	5.879998	-1.545699	-0.056811
22	1	5.787728	-0.477695	-1.498005
23	1	5.875776	0.215607	0.112405
24	1	0.106831	1.683983	-1.787315
25	6	-0.762688	2.718637	0.419954
26	1	-0.861771	3.144858	1.425002
27	1	-0.933439	3.542634	-0.282838
28	1	3.887015	-2.019051	1.209739
29	1	3.519647	1.411420	-0.416354
30	6	1.091110	-0.183800	0.177529
31	1	0.046099	-0.431300	-0.046614
32	6	1.356565	-1.841295	2.112749
33	1	1.673523	-1.073005	2.824156
34	1	0.269597	-1.949317	2.189282
35	1	1.805705	-2.791633	2.420296
36	1	1.350405	-3.616032	0.171088
37	1	0.829114	-2.510252	-1.119953
38	1	1.648847	2.516506	-1.758982
39	1	1.472221	-0.208237	-1.989907
40	6	-1.845122	1.677381	0.228361
41	6	-2.309553	0.914643	1.315141
42	6	-2.437357	1.463955	-1.029193
43	6	-3.288202	-0.063835	1.151916
44	1	-1.918221	1.102243	2.310972
45	6	-3.418061	0.490506	-1.215658
46	1	-2.147800	2.082535	-1.873786
47	6	-3.817439	-0.273029	-0.120596
48	1	-3.652058	-0.649771	1.987358
49	1	-3.878016	0.325204	-2.182496
50	7	-4.837822	-1.322578	-0.309325
51	8	-5.294220	-1.475796	-1.441753
52	8	-5.159220	-1.986931	0.675948

SI-14: TS(C'→F') Bn Analog (X=NO_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1021.55136 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.447405 H
M06-2X/6-31+G(d,p): Electronic Energy: -1021.4867665 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.261248	3.813443	0.173120
2	1	2.007265	4.359475	1.088012
3	1	3.322445	3.547912	0.221911
4	1	2.128371	4.500129	-0.669054
5	6	1.384672	2.560581	0.002461
6	6	1.805396	1.736383	-1.247840
7	6	1.741377	0.222187	-0.898904
8	6	3.115616	-0.495572	-1.199591
9	1	3.377781	-0.252930	-2.235358
10	6	2.902249	-1.965681	-0.955528
11	6	2.938112	-2.365983	0.327845
12	6	1.869378	-3.238197	0.932749
13	1	1.659886	-4.158265	0.381437
14	1	2.092692	-3.522230	1.964905
15	6	0.591027	-2.328700	0.857384
16	6	0.888163	-0.916593	1.376572
17	6	1.623039	1.559725	1.164665
18	1	2.686315	1.570993	1.447115
19	1	1.055002	1.802949	2.063611
20	6	2.323382	-2.767224	-2.092465
21	1	3.074392	-2.855689	-2.887594
22	1	2.043683	-3.780630	-1.797775
23	1	1.448814	-2.287890	-2.553006
24	1	1.191691	1.972243	-2.120722
25	6	-0.104644	3.041990	-0.060440
26	1	-0.287239	3.665385	0.822273
27	1	-0.188473	3.704615	-0.929030
28	1	3.452841	-1.718527	1.039741
29	1	3.896096	-0.077997	-0.552923
30	6	1.350726	0.176851	0.597413
31	1	0.068580	-0.041933	0.754637
32	6	0.721618	-0.789407	2.872591
33	1	0.958550	0.190026	3.281096
34	1	-0.287546	-1.082784	3.176443
35	1	1.405450	-1.517348	3.325813
36	1	-0.234194	-2.746226	1.444479
37	1	0.273895	-2.286293	-0.187379
38	1	2.834385	1.993867	-1.518470
39	1	0.972836	-0.286008	-1.489231
40	6	-1.192307	1.989707	-0.137389
41	6	-1.837430	1.541972	1.032862
42	6	-1.609435	1.451969	-1.369056
43	6	-2.827430	0.559121	0.988364
44	1	-1.585537	1.992075	1.989629
45	6	-2.598623	0.470816	-1.435184
46	1	-1.173076	1.819004	-2.293147
47	6	-3.179940	0.024449	-0.249651
48	1	-3.334772	0.219683	1.883828
49	1	-2.928021	0.059098	-2.381945
50	7	-4.206814	-1.038405	-0.305829
51	8	-4.534437	-1.450335	-1.416130
52	8	-4.650761	-1.450276	0.765084

SI-15: Cation F' Bn Analog (Product; X=NO_2)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1021.600965 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.450986 H
M06-2X/6-31+G(d,p): Electronic Energy: -1021.539232 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.072242	3.490301	0.597647
2	1	1.855459	3.877857	1.598664
3	1	3.140257	3.248548	0.558155
4	1	1.885652	4.298383	-0.117759
5	6	1.210064	2.251524	0.279506
6	6	1.587901	1.671358	-1.106202
7	6	1.387363	0.142109	-1.053629
8	6	2.491327	-0.603967	-1.839329
9	1	2.142220	-1.555345	-2.279006
10	6	3.523449	-0.944410	-0.831711
11	6	2.938321	-1.005371	0.478283
12	6	2.565137	-2.615627	0.453825
13	1	3.100391	-3.202114	-0.299579
14	1	2.901291	-2.974580	1.429009
15	6	1.046230	-2.634782	0.273801
16	6	0.532890	-1.346921	0.940689
17	6	1.547163	1.081885	1.255170
18	1	2.534137	1.261340	1.697605
19	1	0.849676	1.051707	2.093916
20	6	4.941268	-1.175518	-1.148943
21	1	5.391018	-0.169512	-1.229797
22	1	5.480254	-1.708749	-0.363306
23	1	5.083038	-1.647915	-2.125704
24	1	1.034062	2.133658	-1.929631
25	6	-0.279942	2.729524	0.364181
26	1	-0.414221	3.179068	1.354475
27	1	-0.389847	3.546988	-0.358565
28	1	3.618251	-0.826723	1.312875
29	1	2.920039	-0.051370	-2.684600
30	6	1.556475	-0.263063	0.468629
31	1	-0.465065	-1.096278	0.570616
32	6	0.450009	-1.517237	2.467743
33	1	0.012450	-0.644092	2.955969
34	1	-0.187439	-2.372655	2.711714
35	1	1.429586	-1.692956	2.927895
36	1	0.629262	-3.543041	0.722199
37	1	0.778863	-2.665039	-0.788155
38	1	2.648235	1.893188	-1.292959
39	1	0.395772	-0.132603	-1.418849
40	6	-1.403067	1.739451	0.138718
41	6	-2.072973	1.157638	1.228337
42	6	-1.851699	1.426405	-1.157365
43	6	-3.124139	0.260333	1.042527
44	1	-1.784459	1.426118	2.240766
45	6	-2.896337	0.528384	-1.367453
46	1	-1.396089	1.909434	-2.017263
47	6	-3.509324	-0.054733	-0.258908
48	1	-3.647486	-0.184862	1.880252
49	1	-3.249275	0.287987	-2.363161
50	7	-4.604381	-1.022188	-0.470746
51	8	-4.915863	-1.282042	-1.632740
52	8	-5.126576	-1.517309	0.527284

Cation C (4-methylimidazole complex)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.572784 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.465765 H
M06-2X/6-31+G(d,p): Electronic Energy: -851.5667854 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.559632	3.403554	-0.276894
2	1	1.372215	3.543591	0.444288
3	1	0.982940	2.926110	-1.167195
4	1	0.195734	4.396769	-0.562446
5	6	-0.566704	2.555182	0.332910
6	6	-1.686513	2.277677	-0.707448
7	6	-2.408846	1.046886	-0.135902
8	6	-3.270635	0.265471	-1.236042
9	1	-4.145152	0.857192	-1.512985
10	6	-3.583932	-0.989464	-0.563900
11	6	-2.464715	-1.903344	-0.408964
12	6	-2.245322	-2.810282	0.827918
13	1	-2.795630	-2.468810	1.708960
14	1	-2.435544	-3.876084	0.689498
15	6	-0.756548	-2.360921	0.831406
16	6	-1.040851	-1.191365	-0.166437
17	6	-0.084652	1.119109	0.696117
18	1	0.724476	0.819915	0.026181
19	1	0.327994	1.082410	1.709113
20	6	-4.912924	-1.221941	0.028272
21	1	-4.932656	-2.011870	0.778974
22	1	-5.359596	-0.296576	0.409926
23	1	-5.565078	-1.528696	-0.809411
24	1	-2.355425	3.131986	-0.853748
25	6	-1.132224	3.278441	1.572656
26	1	-0.336246	3.458526	2.302796
27	1	-1.912951	2.702260	2.082530
28	1	-1.558197	4.250524	1.300760
29	1	-2.385601	-2.463277	-1.356134
30	1	-2.616871	0.107224	-2.097709
31	6	-1.309484	0.169091	0.548602
32	1	-1.686145	-0.093448	1.546104
33	6	-0.102389	-1.134101	-1.370482
34	1	0.930380	-0.958856	-1.047908
35	1	-0.116053	-2.086527	-1.911498
36	1	-0.367490	-0.341310	-2.078757
37	1	-0.098247	-3.113020	0.389083
38	1	-0.349571	-2.062488	1.800776
39	1	-1.234260	2.036996	-1.677664
40	1	-3.121359	1.378264	0.625958
41	7	5.361182	-0.190013	-1.112089
42	6	5.388982	-0.601303	0.206450
43	6	4.053789	-0.100619	-1.481063
44	1	6.162736	0.005680	-1.693852
45	6	4.073195	-0.744005	0.581270
46	1	6.313128	-0.751933	0.742923
47	1	3.749803	0.201497	-2.473539
48	7	3.248529	-0.426199	-0.486616
49	6	3.524545	-1.171400	1.906640
50	1	4.330965	-1.384518	2.613399
51	1	2.891664	-0.390575	2.343817
52	1	2.915634	-2.077455	1.808047

TS(C→F) (4-methylimidazole complex)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.52865 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.463211 H
M06-2X/6-31+G(d,p): Electronic Energy: -851.5225462 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.694667	3.572610	-0.521763
2	1	1.333295	3.916041	0.299498
3	1	1.325153	3.038893	-1.240999
4	1	0.293154	4.461321	-1.019648
5	6	-0.443160	2.681249	-0.004469
6	6	-1.303425	2.106411	-1.139667
7	6	-2.002753	0.847783	-0.581711
8	6	-2.534284	-0.061087	-1.726703
9	1	-3.110229	0.586100	-2.398602
10	6	-3.344638	-1.133083	-1.061144
11	6	-2.633971	-2.177436	-0.613332
12	6	-2.776279	-2.750303	0.753913
13	1	-3.693275	-2.412671	1.243094
14	1	-2.754872	-3.844895	0.817044
15	6	-1.528215	-2.237156	1.509296
16	6	-0.823236	-0.874792	1.325911
17	6	0.097483	1.385247	0.629442
18	1	0.950124	0.988782	0.056193
19	1	0.460402	1.544927	1.645157
20	6	-4.759853	-0.802496	-0.665223
21	1	-5.210911	-1.569062	-0.031847
22	1	-4.851547	0.165519	-0.155068
23	1	-5.375027	-0.729430	-1.570945
24	1	-2.039721	2.818962	-1.524289
25	6	-1.298618	3.467909	1.009616
26	1	-0.686495	3.813849	1.849561
27	1	-2.121541	2.872624	1.424432
28	1	-1.742930	4.350474	0.538584
29	1	-1.651767	-2.339990	-1.062690
30	1	-1.695160	-0.473113	-2.297206
31	6	-0.994254	0.308301	0.518343
32	1	-1.608780	0.214481	1.639489
33	6	0.412627	-0.878340	2.222692
34	1	0.471061	-0.007888	2.878471
35	1	0.432520	-1.768359	2.850560
36	1	1.298144	-0.874199	1.571630
37	1	-0.693662	-2.908492	1.256126
38	1	-1.652779	-2.362518	2.592447
39	1	-0.660078	1.815693	-1.980282
40	1	-2.879494	1.180600	-0.012984
41	7	4.334323	-1.564028	-1.697681
42	6	5.041044	-0.872718	-0.733562
43	6	3.016565	-1.480821	-1.374471
44	1	4.725853	-2.044167	-2.495231
45	6	4.101795	-0.391853	0.147858
46	1	6.116483	-0.787967	-0.758124
47	1	2.242584	-1.941536	-1.972129
48	7	2.835082	-0.780846	-0.267071
49	6	4.320553	0.423139	1.384500
50	1	5.383711	0.630418	1.530131
51	1	3.798433	1.385019	1.326669
52	1	3.959223	-0.100682	2.277074

Cation C (Bn Analog / 4-methylimidazole complex)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1082.55838 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.547809 H
M06-2X/6-31+G(d,p): Electronic Energy: -1082.538333 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.791044	-2.276775	-2.016549
2	1	-1.365933	-2.975379	-1.399265
3	1	-1.494558	-1.549231	-2.433845
4	1	-0.355146	-2.844962	-2.845671
5	6	0.299275	-1.578654	-1.182740
6	6	1.080215	-0.555831	-2.057225
7	6	1.574422	0.507974	-1.064279
8	6	1.939209	1.900115	-1.775437
9	1	2.870049	1.799514	-2.335505
10	6	2.006518	2.828908	-0.654993
11	6	0.726560	3.166375	-0.056192
12	6	0.523545	3.425798	1.457483
13	1	1.332574	3.023890	2.073293
14	1	0.342966	4.461240	1.751932
15	6	-0.721407	2.493279	1.400345
16	6	-0.333072	1.955086	-0.014491
17	6	-0.338358	-0.687088	-0.067081
18	1	-1.381510	-0.477514	-0.315061
19	1	-0.359622	-1.211661	0.892127
20	6	3.294613	3.209343	-0.048233
21	1	3.207947	4.047864	0.645189
22	1	3.650828	2.337877	0.530967
23	1	4.059742	3.393635	-0.808460
24	1	1.899864	-1.014466	-2.619705
25	6	1.221287	-2.703800	-0.604057
26	1	0.589156	-3.333028	0.034442
27	1	1.530826	-3.335285	-1.445256
28	1	0.289562	3.963999	-0.680168
29	1	1.108152	2.143077	-2.443521
30	6	0.484264	0.628960	0.042076
31	1	1.007175	0.645125	1.007136
32	6	-1.455920	2.001419	-1.048759
33	1	-2.287136	1.358537	-0.738440
34	1	-1.850733	3.019050	-1.141448
35	1	-1.132388	1.674622	-2.043017
36	1	-1.657989	3.055877	1.373534
37	1	-0.786026	1.737580	2.187247
38	1	0.394044	-0.107156	-2.785953
39	1	2.501719	0.158097	-0.605842
40	7	-6.214817	-0.804134	-0.476099
41	6	-5.971997	-1.054663	0.860568
42	6	-5.080197	-0.263857	-0.999668
43	1	-7.075624	-0.985923	-0.971271
44	6	-4.678130	-0.646964	1.088016
45	1	-6.717851	-1.486280	1.510131
46	1	-5.001816	0.028734	-2.037442
47	7	-4.132138	-0.154415	-0.087072
48	6	-3.901385	-0.687925	2.366904
49	1	-4.504494	-1.105293	3.177653
50	1	-3.001794	-1.305520	2.264106
51	1	-3.582689	0.316773	2.667626
52	6	2.460968	-2.304647	0.172066
53	6	3.711836	-2.235485	-0.465268
54	6	2.407583	-2.015896	1.546286
55	6	4.861776	-1.856341	0.232990
56	1	3.790516	-2.500689	-1.517007
57	6	3.553556	-1.634605	2.250078
58	1	1.465460	-2.114547	2.079476
59	6	4.785090	-1.544919	1.593869
60	1	5.819173	-1.826810	-0.279498
61	1	3.489354	-1.432660	3.315650
62	1	5.679638	-1.268070	2.143806

TS(C→F) (Bn Analog / 4-methylimidazole complex)

B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1082.51983 H
B3LYP/6-31+G(d,p) Zero-Point Energy Correction: 0.544949 H
M06-2X/6-31+G(d,p): Electronic Energy: -1082.4981883 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.561854	-2.878631	-2.063441
2	1	-0.923265	-3.676910	-1.405844
3	1	-1.433964	-2.361027	-2.476320
4	1	-0.028237	-3.352518	-2.894020
5	6	0.356168	-1.901191	-1.308454
6	6	0.788666	-0.726231	-2.205579
7	6	1.013599	0.518398	-1.313100
8	6	0.718738	1.831953	-2.104049
9	1	1.204938	1.730635	-3.081452
10	6	1.277487	2.935178	-1.254457
11	6	0.476630	3.341648	-0.259120
12	6	0.925413	3.476120	1.156503
13	1	2.014661	3.449932	1.237926
14	1	0.578404	4.372079	1.685520
15	6	0.285223	2.261232	1.873109
16	6	-0.028355	0.879462	1.254216
17	6	-0.421410	-1.165873	-0.199990
18	1	-1.446192	-0.936177	-0.530190
19	1	-0.526792	-1.765697	0.702848
20	6	2.754841	3.210890	-1.352298
21	1	3.107484	3.893943	-0.576800
22	1	3.365405	2.299295	-1.314766
23	1	2.965307	3.684022	-2.319813
24	1	1.681166	-0.945493	-2.799780
25	6	1.556516	-2.731338	-0.745724
26	1	1.133508	-3.541490	-0.138931
27	1	2.043025	-3.212574	-1.601844
28	1	-0.591935	3.144318	-0.369937
29	1	-0.358035	1.938436	-2.274549
30	6	0.229343	0.204142	0.017212
31	1	1.083323	0.096560	0.975256
32	6	-0.885852	0.115210	2.260573
33	1	-0.513619	-0.890265	2.462866
34	1	-0.936399	0.647259	3.210274
35	1	-1.896684	0.029362	1.839429
36	1	-0.728744	2.566076	2.167615
37	1	0.790210	2.054805	2.826256
38	1	-0.017742	-0.506706	-2.916135
39	1	2.068756	0.552585	-1.027038
40	7	-5.713338	0.874585	-0.475153
41	6	-5.949691	-0.370003	0.074412
42	6	-4.384610	1.131543	-0.343340
43	1	-6.402042	1.482622	-0.894421
44	6	-4.730091	-0.820015	0.522533
45	1	-6.934116	-0.811276	0.098639
46	1	-3.933723	2.049219	-0.694138
47	7	-3.756632	0.132443	0.253116
48	6	-4.411936	-2.113981	1.205185
49	1	-5.312577	-2.721246	1.326576
50	1	-3.688619	-2.702189	0.628873
51	1	-3.987687	-1.945783	2.201749
52	6	2.612090	-2.015326	0.074541
53	6	3.778391	-1.509883	-0.523549
54	6	2.474208	-1.872147	1.467906
55	6	4.755847	-0.858327	0.233608
56	1	3.934279	-1.647127	-1.590719
57	6	3.448995	-1.218201	2.231214
58	1	1.623146	-2.327942	1.969892
59	6	4.590479	-0.700502	1.613122
60	1	5.655196	-0.489672	-0.250946
61	1	3.331453	-1.143150	3.308637
62	1	5.356900	-0.207857	2.203334

Additional C-H···N Complexes with 4-methylimidazole

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.586142 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.747875	3.359837	0.030381
2	1	-0.464868	3.723565	1.024593
3	1	0.126337	2.852934	-0.396673
4	1	-0.961848	4.234295	-0.593979
5	6	-1.969062	2.426778	0.113264
6	6	-2.342433	1.818875	-1.289391
7	6	-2.140870	0.290541	-1.184050
8	6	-0.712643	-0.109962	-1.606040
9	1	-0.583383	-0.072338	-2.694950
10	6	-0.161177	-1.372357	-1.060887
11	6	-0.846803	-2.057824	0.006895
12	6	-1.900116	-3.027674	-0.779623
13	1	-2.034461	-2.786915	-1.836565
14	1	-1.605555	-4.074052	-0.692239
15	6	-3.013225	-2.498274	0.146869
16	6	-2.060092	-1.425307	0.772542
17	6	-1.671582	1.179066	1.004524
18	1	-0.590046	0.989979	1.052385
19	1	-2.004710	1.330578	2.035186
20	6	1.092741	-1.889275	-1.579255
21	1	1.298140	-2.924539	-1.299325
22	1	1.231756	-1.718819	-2.650316
23	1	1.891864	-1.248126	-1.074304
24	1	-3.390178	2.030504	-1.525227
25	6	-3.165287	3.215582	0.681834
26	1	-2.919807	3.654621	1.655065
27	1	-4.045855	2.576282	0.814042
28	1	-3.449128	4.032262	0.008825
29	1	-0.178114	-2.670654	0.615994
30	1	0.017533	0.633564	-1.231345
31	6	-2.399495	0.005922	0.316073
32	1	-3.476439	0.136986	0.490933
33	6	-1.926529	-1.548470	2.291824
34	1	-1.113334	-0.928649	2.681766
35	1	-2.855878	-1.234789	2.780034
36	1	-1.732851	-2.585111	2.588214
37	1	-3.347835	-3.244952	0.871220
38	1	-3.889006	-2.102856	-0.374249
39	1	-1.748146	2.257089	-2.099484
40	1	-2.847930	-0.247320	-1.826371
41	1	5.955630	1.566770	-0.847825
42	7	5.193309	1.015211	-0.480161
43	6	5.059979	0.573404	0.821664
44	6	4.119880	0.567487	-1.178516
45	6	3.885460	-0.139123	0.861034
46	1	5.791431	0.796140	1.582929
47	1	3.979097	0.768269	-2.231020
48	6	3.258263	-0.844512	2.022124
49	1	2.266859	-0.435584	2.248721
50	1	3.144361	-1.915922	1.821591
51	1	3.873951	-0.738300	2.918638
52	7	3.307779	-0.129953	-0.400391

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.58309 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.473996	-1.767838	1.040554
2	1	-4.457320	-2.794241	0.657319
3	1	-3.802207	-1.723213	1.906038
4	1	-5.488952	-1.565064	1.398711
5	6	-4.064496	-0.764095	-0.050978
6	6	-4.001074	0.708965	0.497255
7	6	-2.543695	1.194898	0.344429
8	6	-1.684026	0.934947	1.638095
9	1	-1.591004	1.886987	2.178806
10	6	-0.314681	0.409277	1.347199
11	6	0.537975	1.028142	0.444289
12	6	0.364113	2.399895	-0.193462
13	1	-0.394050	3.010624	0.299987
14	1	1.300676	2.960553	-0.210118
15	6	-0.087220	1.875760	-1.569263
16	6	-0.525926	0.463279	-1.120819
17	6	-2.616700	-1.048392	-0.561450
18	1	-2.040684	-1.577408	0.206926
19	1	-2.617178	-1.687238	-1.449882
20	6	0.125928	-0.849409	2.024851
21	1	1.055292	-1.245329	1.611237
22	1	0.312594	-0.599901	3.080843
23	1	-0.653530	-1.617109	2.029540
24	1	-4.664818	1.356328	-0.085263
25	6	-5.067755	-0.849536	-1.218315
26	1	-5.126287	-1.869716	-1.613285
27	1	-6.071908	-0.561109	-0.889400
28	1	1.514497	0.561166	0.295910
29	1	-2.202476	0.243903	2.306728
30	6	-2.006424	0.338378	-0.829713
31	1	-2.470535	0.742288	-1.745818
32	6	0.162449	-0.708034	-1.762943
33	1	-0.054752	-1.653092	-1.260692
34	1	-0.223622	-0.783941	-2.791261
35	1	1.243619	-0.565465	-1.820322
36	1	0.748279	1.808297	-2.270738
37	1	-0.896111	2.439994	-2.043836
38	1	-4.339417	0.776338	1.536311
39	1	-2.509249	2.261948	0.110547
40	1	4.157305	2.219544	-0.388919
41	6	4.617381	1.664770	0.437180
42	6	4.668192	0.197894	0.143243
43	1	4.038002	1.870047	1.344793
44	1	5.622438	2.067216	0.586931
45	6	5.771987	-0.616606	0.051143
46	7	3.521143	-0.548635	-0.086949
47	7	5.287425	-1.876506	-0.239537
48	1	6.826542	-0.416796	0.162206
49	6	3.933096	-1.784987	-0.312271
50	1	5.839001	-2.711501	-0.375381
51	1	3.304951	-2.637076	-0.531435
52	1	-4.789850	-0.184904	-2.045229

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.584071 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.670069	3.583892	0.371080
2	1	1.667112	3.951549	1.403380
3	1	2.678435	3.214923	0.151351
4	1	1.479663	4.439789	-0.285170
5	6	0.603918	2.492266	0.171537
6	6	0.641535	1.889183	-1.281603
7	6	1.057735	0.406383	-1.164442
8	6	2.610336	0.224948	-1.279124
9	1	2.834861	0.019292	-2.335228
10	6	3.258609	-0.838648	-0.421708
11	6	2.810618	-2.118894	-0.346988
12	6	1.612421	-2.692929	-1.082180
13	1	1.455287	-2.189507	-2.038586
14	1	1.759127	-3.754095	-1.297733
15	6	0.407128	-2.487556	-0.133790
16	6	0.780923	-1.312957	0.752804
17	6	0.872460	1.269991	1.108056
18	1	1.926437	1.246667	1.411526
19	1	0.276594	1.323986	2.024635
20	6	4.483411	-0.416098	0.349029
21	1	4.891069	-1.225914	0.958722
22	1	5.266167	-0.092787	-0.349262
23	1	4.275314	0.443678	0.996574
24	1	-0.352822	1.954677	-1.734895
25	6	-0.789483	3.086438	0.456263
26	1	-0.835663	3.513891	1.464150
27	1	-1.020345	3.887054	-0.255038
28	1	3.349359	-2.805986	0.304208
29	1	3.094830	1.179104	-1.055853
30	6	0.541750	0.036709	0.256684
31	1	-0.579078	-0.042019	0.125565
32	6	0.975862	-1.556771	2.202664
33	1	1.592239	-0.796584	2.685414
34	1	-0.029160	-1.493932	2.657544
35	1	1.355160	-2.558262	2.412949
36	1	0.247802	-3.374294	0.486016
37	1	-0.528524	-2.267803	-0.660938
38	1	1.323170	2.441458	-1.936576
39	1	0.563022	-0.197780	-1.928463
40	1	-2.846479	-1.584580	2.253579
41	6	-3.382501	-0.651317	2.042939
42	6	-3.642083	-0.491822	0.577485
43	1	-2.784866	0.179965	2.434193
44	1	-4.320334	-0.677448	2.603236
45	6	-4.850811	-0.417788	-0.072998
46	7	-2.615032	-0.396072	-0.350960
47	7	-4.551078	-0.274404	-1.413039
48	1	-5.866555	-0.451734	0.289436
49	6	-3.198421	-0.266018	-1.531601
50	1	-5.217231	-0.190017	-2.167743
51	1	-2.697120	-0.162046	-2.483418
52	1	-1.575555	2.328009	0.369784

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.54626 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.646601	-3.326142	-1.185183
2	1	2.298228	-4.192411	-0.612301
3	1	1.983846	-3.201161	-2.048421
4	1	3.647278	-3.561528	-1.561732
5	6	2.677983	-2.060979	-0.317306
6	6	3.118046	-0.804079	-1.113649
7	6	2.375090	0.424205	-0.512173
8	6	1.675391	1.281088	-1.638137
9	1	2.447730	1.520926	-2.377500
10	6	1.076448	2.490292	-0.968140
11	6	-0.088693	2.292277	-0.325458
12	6	-0.323828	2.770376	1.084384
13	1	-0.109526	3.828515	1.254860
14	1	-1.343814	2.577678	1.427213
15	6	0.712785	1.927737	1.907577
16	6	0.625885	0.442054	1.535056
17	6	1.257281	-1.655959	0.154765
18	1	0.544232	-1.721590	-0.681200
19	1	0.866718	-2.285674	0.955179
20	6	1.982662	3.677797	-0.769352
21	1	2.191550	4.139137	-1.742865
22	1	1.539171	4.447069	-0.133671
23	1	2.959606	3.403794	-0.348533
24	1	4.203235	-0.668529	-1.096973
25	6	3.595999	-2.286537	0.900710
26	1	3.231650	-3.108018	1.527245
27	1	3.686284	-1.394866	1.535990
28	1	4.608556	-2.541510	0.573018
29	1	-0.674792	1.415273	-0.602438
30	1	0.915382	0.669004	-2.136845
31	6	1.365431	-0.185347	0.492493
32	1	1.809035	-0.103362	1.745784
33	6	-0.463948	-0.312242	2.253162
34	1	-0.288786	-1.384716	2.332906
35	1	-0.635067	0.099661	3.248898
36	1	-1.375730	-0.178012	1.644544
37	1	0.545815	2.022520	2.985585
38	1	1.708891	2.317315	1.683046
39	1	2.828014	-0.915085	-2.164258
40	1	3.066300	1.085625	0.020703
41	7	-4.847362	0.360739	-1.090511
42	6	-4.964172	-0.964561	-0.720771
43	6	-3.637009	0.800037	-0.654760
44	1	-5.536170	0.904212	-1.590542
45	6	-3.796347	-1.275180	-0.064820
46	1	-5.840993	-1.550875	-0.948356
47	1	-3.292981	1.811746	-0.818143
48	7	-2.972420	-0.158743	-0.031947
49	6	-3.396712	-2.580173	0.550022
50	1	-4.177017	-3.332125	0.407588
51	1	-2.475086	-2.967020	0.099858
52	1	-3.226449	-2.477949	1.628047

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -851.547133 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.860340	3.596391	-1.115359
2	1	-1.405236	4.372692	-0.490671
3	1	-1.169678	3.372709	-1.935748
4	1	-2.772479	4.017369	-1.550578
5	6	-2.181426	2.339203	-0.295646
6	6	-2.788817	1.205098	-1.164753
7	6	-2.310437	-0.155271	-0.578598
8	6	-1.677573	-1.071624	-1.695481
9	1	-2.419955	-1.151630	-2.497525
10	6	-1.336236	-2.389067	-1.049279
11	6	-0.202569	-2.418051	-0.325160
12	6	-0.150648	-2.982299	1.072001
13	1	-0.543167	-3.996990	1.178160
14	1	0.859895	-2.972815	1.489242
15	6	-1.095944	-2.012005	1.864949
16	6	-0.736932	-0.551101	1.571647
17	6	-0.895822	1.669444	0.253757
18	1	-0.118321	1.625980	-0.523887
19	6	-2.437882	-3.414415	-0.972250
20	1	-2.645960	-3.796177	-1.979835
21	1	-2.176660	-4.271604	-0.348062
22	1	-3.385323	-2.996499	-0.605788
23	1	-3.880078	1.265032	-1.208033
24	6	-3.125575	2.703948	0.867346
25	1	-2.661110	3.431076	1.542359
26	1	-3.420833	1.831595	1.466486
27	1	-4.049417	3.148157	0.484229
28	1	0.534849	-1.638063	-0.517886
29	1	-0.792645	-0.574963	-2.109196
30	6	-1.289057	0.233373	0.519947
31	1	-1.834191	0.184611	1.726891
32	6	0.409557	-0.008647	2.388781
33	1	0.337032	1.059438	2.596206
34	1	0.509414	-0.547893	3.331402
35	1	1.317273	-0.155015	1.779998
36	1	-1.030982	-2.174930	2.945830
37	1	-2.120751	-2.220876	1.548907
38	1	-2.425047	1.296299	-2.193916
39	1	-3.141392	-0.709197	-0.129761
40	7	4.672599	-0.615651	-1.130272
41	6	4.866061	0.670923	-0.668203
42	6	3.434772	-1.010210	-0.730648
43	1	5.331830	-1.164131	-1.663671
44	6	3.713887	1.005192	0.003574
45	1	5.778404	1.217531	-0.850587
46	1	3.033655	-1.986578	-0.963930
47	7	2.823292	-0.058804	-0.044732
48	6	3.390925	2.286629	0.706909
49	1	4.220613	2.993588	0.626873
50	1	2.503603	2.765731	0.277116
51	1	3.198769	2.119727	1.773069
52	1	-0.459018	2.191941	1.106125

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1082.573299 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.111646	-2.798923	-0.759496
2	1	-0.005088	-3.377797	0.163696
3	1	-0.871316	-2.385474	-1.014974
4	1	0.391653	-3.496809	-1.556145
5	6	1.173306	-1.693676	-0.590378
6	6	1.265124	-0.790906	-1.871692
7	6	0.753019	0.611099	-1.474070
8	6	-0.766530	0.741724	-1.703371
9	1	-1.008765	0.877441	-2.765221
10	6	-1.508026	1.722549	-0.876584
11	6	-0.862887	2.360954	0.242333
12	6	-0.155370	3.668354	-0.440769
13	1	-0.113946	3.644954	-1.531877
14	1	-0.656811	4.584916	-0.127894
15	6	1.157492	3.272231	0.263393
16	6	0.546921	1.920559	0.765916
17	6	0.763810	-0.703012	0.545912
18	1	-0.316773	-0.777044	0.733629
19	1	1.256080	-0.932612	1.493588
20	6	-2.901128	2.010730	-1.180913
21	1	-3.281392	2.912227	-0.695570
22	1	-3.128205	1.995410	-2.250426
23	1	-3.482097	1.135799	-0.741606
24	1	2.300980	-0.700718	-2.205246
25	6	2.530832	-2.417788	-0.292854
26	1	2.357414	-3.100446	0.547964
27	1	2.754658	-3.051156	-1.160125
28	1	-1.567875	2.691854	1.008633
29	1	-1.281141	-0.203910	-1.444611
30	6	1.128249	0.702568	0.024816
31	1	2.219818	0.797224	0.080087
32	6	0.589627	1.770571	2.287911
33	1	-0.011354	0.924320	2.633518
34	1	1.621478	1.613737	2.620437
35	1	0.216583	2.673501	2.783859
36	1	1.418856	3.951967	1.078292
37	1	2.020052	3.178042	-0.401137
38	1	0.701180	-1.215539	-2.710350
39	1	1.251552	1.390856	-2.061955
40	1	-7.441761	-1.788684	-0.427486
41	7	-6.543232	-1.432571	-0.133832
42	6	-5.918862	-1.686061	1.071964
43	6	-5.734609	-0.611921	-0.850569
44	6	-4.731214	-0.995121	1.034768
45	1	-6.360580	-2.316801	1.827737
46	1	-5.988082	-0.254364	-1.838408
47	6	-3.663215	-0.918657	2.080593
48	1	-2.718126	-1.337922	1.716637
49	1	-3.478193	0.118164	2.385380
50	1	-3.954054	-1.479311	2.972412
51	7	-4.630392	-0.330181	-0.178645
52	6	3.745900	-1.565831	0.017703
53	6	4.056404	-1.204337	1.339649
54	6	4.619923	-1.145174	-0.998867
55	6	5.175222	-0.420157	1.632797
56	1	3.431716	-1.562913	2.154215
57	6	5.740054	-0.359862	-0.712497
58	1	4.441550	-1.459339	-2.024342
59	6	6.017435	0.013124	0.605072
60	1	5.399961	-0.165386	2.664627
61	1	6.405116	-0.056458	-1.515896
62	1	6.893537	0.613314	0.831278

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1082.570878 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.068377	3.016294	-1.298824
2	1	3.106421	2.920738	-2.389802
3	1	2.233894	3.682167	-1.050926
4	1	3.991164	3.510265	-0.976426
5	6	2.911795	1.640641	-0.623800
6	6	2.736769	1.784783	0.930990
7	6	1.339247	1.239190	1.296498
8	6	0.237932	2.361521	1.328845
9	1	0.065677	2.636976	2.378090
10	6	-1.065509	1.953723	0.708146
11	6	-1.745501	0.814892	1.085275
12	6	-1.392448	-0.126289	2.223522
13	1	-0.728407	0.327884	2.961427
14	1	-2.284382	-0.486270	2.739787
15	6	-0.691130	-1.204522	1.375912
16	6	-0.331278	-0.365816	0.133226
17	6	1.596711	0.944617	-1.096198
18	1	0.887663	1.699560	-1.455000
19	1	1.766463	0.253814	-1.925886
20	6	-1.630159	2.823626	-0.376066
21	1	-2.498394	2.375803	-0.863429
22	1	-1.954755	3.768221	0.083992
23	1	-0.878390	3.092926	-1.124447
24	1	3.496385	1.204171	1.459098
25	6	4.184671	0.801662	-0.984865
26	1	4.307968	0.848205	-2.073571
27	1	5.048454	1.323782	-0.556012
28	1	-2.677909	0.586143	0.564773
29	1	0.604947	3.260304	0.827704
30	6	1.045896	0.236601	0.152860
31	1	1.686326	-0.643115	0.342783
32	6	-0.914790	-0.787341	-1.178970
33	1	-0.797638	-0.030671	-1.957533
34	1	-0.350169	-1.678266	-1.498421
35	1	-1.965539	-1.071598	-1.087029
36	1	-1.381803	-2.004191	1.097175
37	1	0.193250	-1.653350	1.839405
38	1	2.858657	2.823201	1.256196
39	1	1.360785	0.738227	2.267549
40	6	4.222969	-0.652960	-0.556331
41	6	3.761314	-1.668122	-1.412533
42	6	4.750719	-1.036704	0.688584
43	6	3.788563	-3.011027	-1.026084
44	1	3.405165	-1.409321	-2.406884
45	6	4.779510	-2.377950	1.081277
46	1	5.174164	-0.283659	1.348326
47	6	4.290012	-3.370409	0.228186
48	1	3.441228	-3.777362	-1.713285
49	1	5.203895	-2.648123	2.043871
50	1	4.325009	-4.414100	0.525440
51	1	-4.666818	-1.827437	1.962669
52	6	-5.433413	-1.074482	1.745546
53	6	-5.577418	-0.855504	0.271824
54	1	-5.152312	-0.148141	2.259923
55	1	-6.373091	-1.423388	2.181253
56	6	-6.692796	-1.034711	-0.511960
57	7	-4.523513	-0.414443	-0.515975
58	7	-6.310157	-0.696651	-1.794906
59	1	-7.693703	-1.362487	-0.277185
60	6	-5.001641	-0.331188	-1.746066
61	1	-6.895470	-0.717699	-2.617570
62	1	-4.453466	-0.018692	-2.623864

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -1082.538588 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.462692	-2.664378	2.648656
2	1	-0.221915	-3.601228	2.134554
3	1	0.458789	-2.278295	3.097257
4	1	-1.156120	-2.902768	3.461942
5	6	-1.081897	-1.638662	1.684371
6	6	-1.344418	-0.278138	2.394687
7	6	-0.963948	0.874988	1.422945
8	6	0.111490	1.834623	2.065242
9	1	-0.285479	2.151706	3.036195
10	6	0.323934	2.970531	1.097862
11	6	1.118760	2.710122	0.044129
12	6	0.719196	3.033649	-1.373006
13	1	0.403710	4.066917	-1.539987
14	1	1.513095	2.810437	-2.091140
15	6	-0.524324	2.102343	-1.598321
16	6	-0.217964	0.671605	-1.144788
17	6	-0.081493	-1.250940	0.566051
18	1	0.942988	-1.192726	0.962854
19	1	-0.049559	-1.964101	-0.258856
20	6	-0.633099	4.130987	1.190016
21	1	-0.444959	4.682621	2.119826
22	1	-0.521197	4.837493	0.364685
23	1	-1.684179	3.814264	1.232006
24	1	-2.378661	-0.190132	2.736725
25	6	-2.388011	-2.270263	1.097961
26	1	-2.127714	-3.261635	0.708553
27	1	-3.068883	-2.440377	1.940084
28	1	1.795337	1.859491	0.129924
29	1	1.033913	1.272204	2.249387
30	6	-0.435509	0.162770	0.158465
31	1	-1.363634	0.077929	-0.789829
32	6	0.521144	-0.173421	-2.157158
33	1	0.187373	-1.212355	-2.173681
34	1	0.416907	0.241154	-3.160437
35	1	1.581238	-0.177279	-1.864208
36	1	-0.824596	2.074654	-2.651022
37	1	-1.356269	2.511900	-1.020413
38	1	-0.717039	-0.210395	3.289392
39	1	-1.837124	1.481516	1.165614
40	7	5.709426	0.024776	-0.013442
41	6	5.588072	-1.309055	-0.348860
42	6	4.464986	0.570624	-0.058381
43	1	6.565853	0.506753	0.219072
44	6	4.249459	-1.515250	-0.586213
45	1	6.438111	-1.972520	-0.389645
46	1	4.280700	1.612671	0.162691
47	7	3.555711	-0.327311	-0.399110
48	6	3.566249	-2.784154	-0.991744
49	1	4.286820	-3.600629	-1.085548
50	1	2.814577	-3.086940	-0.253679
51	1	3.061009	-2.673862	-1.958228
52	6	-3.122441	-1.508366	0.010610
53	6	-2.908064	-1.813706	-1.346562
54	6	-4.060470	-0.506010	0.317084
55	6	-3.578782	-1.121845	-2.361117
56	1	-2.235254	-2.626502	-1.610691
57	6	-4.733887	0.187159	-0.692507
58	1	-4.289700	-0.284737	1.355924
59	6	-4.489130	-0.111944	-2.036398
60	1	-3.408908	-1.389149	-3.400068
61	1	-5.465006	0.945882	-0.429241
62	1	-5.023129	0.416159	-2.820287

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MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.096620 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.861719	-0.921250	1.417495
2	1	-2.263089	-1.934408	1.393594
3	1	-0.800047	-0.977963	1.647274
4	1	-2.371164	-0.374141	2.213082
5	6	-2.091170	-0.264795	0.045943
6	6	-1.908597	1.199630	0.128235
7	6	-1.078729	2.055324	-0.617813
8	1	-1.423406	3.070796	-0.773984
9	6	-0.068987	2.114443	0.763521
10	1	-0.160093	3.171449	1.014277
11	6	1.280630	1.605711	0.399885
12	6	1.715551	0.493861	1.039895
13	6	2.885189	-0.360555	0.663659
14	1	3.778547	0.226847	0.444529
15	1	3.132635	-1.020373	1.495713
16	6	2.509146	-1.204329	-0.597936
17	6	1.075084	-1.669864	-0.534799
18	6	-1.356130	-1.014897	-1.094623
19	1	-1.660788	-2.060623	-1.001570
20	1	-1.766975	-0.664983	-2.046961
21	6	2.037859	2.323318	-0.681295
22	1	1.981385	3.404452	-0.540776
23	1	3.088783	2.042276	-0.669329
24	1	1.650265	2.101631	-1.679538
25	1	-2.558842	1.688729	0.854270
26	6	-3.626886	-0.321808	-0.258351
27	1	-3.875937	-1.373671	-0.402719
28	1	-3.887328	0.216063	-1.170908
29	1	-4.218301	0.063887	0.571864
30	1	1.069180	0.087700	1.812745
31	1	-0.460584	1.549469	1.617100
32	1	-0.535714	1.628322	-1.447680
33	6	0.140464	-0.898404	-1.136828
34	1	0.529654	-0.092676	-1.752529
35	6	0.795807	-2.886098	0.300353
36	1	1.406445	-3.720680	-0.049084
37	1	1.063375	-2.718674	1.348107
38	1	-0.247764	-3.192570	0.262635
39	1	3.201070	-2.045293	-0.682198
40	1	2.643624	-0.577288	-1.481958

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MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.089909 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.507728	0.553185	1.252004
2	1	3.227559	1.321486	0.971885
3	1	1.607930	1.045104	1.618166
4	1	2.937252	-0.042451	2.058919
5	6	2.219236	-0.328860	0.016273
6	6	1.203599	-1.301962	0.482981
7	6	0.208803	-1.972937	-0.250773
8	1	1.117588	-2.732981	-0.133836
9	6	-1.059883	-2.463315	0.423690
10	1	-1.441144	-3.352714	-0.076541
11	6	-2.031622	-1.289375	0.286103
12	6	-1.758647	-0.153204	0.959478
13	6	-2.415428	1.187627	0.790879
14	1	-3.497623	1.094093	0.683937
15	1	-2.240289	1.790834	1.683571
16	6	-1.850095	1.918714	-0.460758
17	6	-0.340045	1.909912	-0.482371
18	6	1.733564	0.526635	-1.191758
19	1	2.382587	1.405590	-1.223945
20	1	1.928600	-0.026546	-2.114949
21	6	-3.146934	-1.464861	-0.702810
22	1	-3.748442	-2.339847	-0.448957
23	1	-3.803689	-0.598393	-0.729067
24	1	-2.756936	-1.624384	-1.712937
25	1	1.262145	-1.590828	1.535164
26	6	3.513516	-1.098058	-0.348260
27	1	4.275928	-0.362913	-0.606833
28	1	3.353838	-1.748334	-1.209260
29	1	3.881734	-1.691032	0.489979
30	1	-0.895429	-0.165915	1.627394
31	1	-0.866853	-2.713330	1.469364
32	1	0.140556	-1.742908	-1.308506
33	6	0.275397	0.907998	-1.152417
34	1	-0.384913	0.271960	-1.733995
35	6	0.348299	2.995940	0.294758
36	1	-0.013842	3.967157	-0.048012
37	1	0.121136	2.937261	1.362971
38	1	1.429287	2.980420	0.171897
39	1	-2.234099	2.941690	-0.476302
40	1	-2.227802	1.412348	-1.352225

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MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.125231 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.570582	0.361881	-0.651276
2	1	-4.182193	1.064997	-0.084444
3	1	-3.384040	0.795186	-1.636406
4	1	-4.146372	-0.556361	-0.783394
5	6	-2.254267	0.086436	0.088075
6	6	-1.392292	-0.787384	-0.857525
7	6	-0.398140	-1.755411	-0.270345
8	6	0.479195	-2.568962	-1.061906
9	1	0.672674	-3.594073	-0.767128
10	6	1.350743	-1.604732	-0.175896
11	6	1.766403	-0.435998	-0.757661
12	6	2.869252	0.429879	-0.267365
13	1	3.653796	-0.156695	0.212126
14	1	3.301830	0.960575	-1.116034
15	6	2.275506	1.457602	0.751801
16	6	0.917341	1.913072	0.281204
17	6	-1.591895	1.453589	0.381336
18	1	-1.653776	2.063437	-0.522323
19	1	-2.198776	1.955687	1.143079
20	6	1.966406	-2.178325	1.073348
21	1	2.974431	-2.536858	0.860423
22	1	2.018408	-1.435721	1.867942
23	1	1.385189	-3.025007	1.435799
24	1	-2.078831	-1.473925	-1.375969
25	6	-2.575552	-0.648580	1.392654
26	1	-3.323374	-0.085471	1.952167
27	1	-1.706414	-0.763510	2.043100
28	1	-2.993092	-1.639898	1.196901
29	1	1.237437	-0.102470	-1.646253
30	1	0.525916	-2.380181	-2.127924
31	1	-0.609283	-2.114053	0.731705
32	6	-0.173685	1.336041	0.834495
33	1	0.000482	0.684262	1.689466
34	6	0.913083	2.900055	-0.853507
35	1	1.467582	3.794020	-0.560710
36	1	1.412473	2.500854	-1.741771
37	1	-0.087894	3.210514	-1.141170
38	1	2.983999	2.282894	0.849085
39	1	2.187405	0.975252	1.726641
40	1	-0.946677	-0.178434	-1.649506

SI-27

MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.106885 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.797146	0.305559	-0.697066
2	1	-4.411864	0.977405	-0.096812
3	1	-3.563455	0.810084	-1.636551
4	1	-4.392126	-0.581787	-0.920387
5	6	-2.522696	-0.060542	0.065217
6	6	-1.610204	-0.878755	-0.852371
7	6	-0.391942	-1.414736	-0.263416
8	6	0.718150	-2.022860	-1.011331
9	1	0.691921	-3.108213	-0.841139
10	6	1.939371	-1.403545	-0.342297
11	6	2.373865	-0.237140	-0.864017
12	6	3.140136	0.795377	-0.113725
13	1	3.979130	0.393145	0.454243
14	1	3.538098	1.552348	-0.788053
15	6	2.120428	1.429642	0.898736
16	6	0.751472	1.605043	0.318999
17	6	-1.748005	1.225568	0.437928
18	1	-1.766619	1.903769	-0.416593
19	1	-2.290818	1.724340	1.248212
20	6	2.420668	-2.038680	0.927988
21	1	2.682496	-3.083383	0.748231
22	1	3.303500	-1.534167	1.314056
23	1	1.660765	-2.026497	1.714699
24	1	-2.132483	-1.827536	-1.111311
25	6	-2.895542	-0.851659	1.322601
26	1	-3.636071	-0.293744	1.896387
27	1	-2.048809	-1.030829	1.987473
28	1	-3.337401	-1.816498	1.063412
29	1	1.913304	0.092507	-1.792784
30	1	0.668145	-1.817283	-2.080076
31	6	-0.336466	0.969495	0.865262
32	1	-0.175372	0.445874	1.805079
33	6	0.633241	2.530371	-0.863002
34	1	0.134839	3.457872	-0.570765
35	1	1.613300	2.793912	-1.255389
36	1	0.050138	2.091371	-1.674469
37	1	2.507350	2.406484	1.208973
38	1	2.063547	0.793377	1.784263
39	1	-1.411358	-0.394621	-1.814313
40	1	-0.412144	-1.646773	0.796578

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MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.147369 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.849734	-0.362262	-0.492909
2	1	4.344672	-1.149915	0.077781
3	1	3.669523	-0.734872	-1.503067
4	1	4.534495	0.485132	-0.556530
5	6	2.542720	0.043397	0.182760
6	6	1.780827	1.086632	-0.658203
7	6	0.351701	1.014156	-0.084487
8	6	-0.701317	1.475829	-1.226866
9	1	-0.494927	2.505778	-1.506236
10	6	-1.846879	1.263467	-0.398064
11	6	-2.256953	-0.128534	-0.222088
12	6	-2.747826	-0.701205	1.128401
13	1	-2.361829	-0.133533	1.975916
14	1	-3.820269	-0.837425	1.252116
15	6	-1.893253	-1.955885	0.830304
16	6	-1.068928	-1.166045	-0.223153
17	6	1.525997	-1.111787	0.221238
18	1	1.569637	-1.637352	-0.734806
19	1	1.746212	-1.838209	1.006746
20	6	-2.483635	2.364100	0.342845
21	1	-3.442622	2.525107	-0.172727
22	1	-2.732669	2.086872	1.366119
23	1	-1.918378	3.291774	0.301608
24	1	2.204156	2.091237	-0.595213
25	6	2.832822	0.574998	1.589309
26	1	3.352507	-0.184080	2.176012
27	1	1.926118	0.846043	2.134419
28	1	3.472776	1.457936	1.541482
29	1	-2.948294	-0.361826	-1.047055
30	1	-0.591924	0.775359	-2.049471
31	6	0.147630	-0.447067	0.413749
32	1	-0.061570	-0.386259	1.487266
33	6	-0.785769	-1.915481	-1.515771
34	1	-0.215531	-2.821069	-1.305092
35	1	-1.723129	-2.221726	-1.982819
36	1	-0.218027	-1.331218	-2.242397
37	1	-2.487337	-2.736342	0.352211
38	1	-1.334707	-2.389113	1.660265
39	1	1.782747	0.774765	-1.707081
40	1	0.267134	1.717069	0.748171

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MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.118133 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.887435	-0.351819	-0.744530
2	1	-4.433627	0.588654	-0.834889
3	1	-3.679499	-0.727981	-1.747650
4	1	-4.537111	-1.068282	-0.240228
5	6	-2.596558	-0.160286	0.043626
6	6	-1.769903	-1.453878	0.156344
7	6	-0.286540	-1.030379	0.283771
8	6	0.633311	-1.821649	-0.707837
9	1	0.465719	-2.885860	-0.523480
10	6	2.031386	-1.362468	-0.428542
11	6	2.399488	-0.185594	-0.985222
12	6	3.096445	0.875432	-0.184427
13	1	4.001137	0.541740	0.323008
14	1	3.360488	1.743814	-0.788421
15	6	2.029889	1.234444	0.893845
16	6	0.683746	1.462149	0.214771
17	6	-1.612575	0.770986	-0.692081
18	1	-1.526986	0.465768	-1.744752
19	1	-1.894456	1.823179	-0.667290
20	6	2.753859	-2.034368	0.704206
21	1	2.968777	-3.067901	0.423864
22	1	3.702661	-1.553448	0.933733
23	1	2.156415	-2.077600	1.619459
24	1	-2.090208	-2.074710	0.994718
25	6	-2.908943	0.402911	1.433132
26	1	-3.370557	1.389899	1.362662
27	1	-2.017872	0.487182	2.064781
28	1	-3.602077	-0.256242	1.956830
29	1	1.828751	0.165505	-1.843414
30	1	0.324349	-1.602606	-1.734776
31	6	-0.287387	0.462852	-0.051722
32	1	-0.217000	1.237045	1.068444
33	6	0.500817	2.849732	-0.377580
34	1	-0.004390	2.820303	-1.339349
35	1	-0.054582	3.505875	0.293949
36	1	1.485813	3.290733	-0.514682
37	1	2.289468	2.137141	1.453276
38	1	1.964877	0.402252	1.595696
39	1	-1.893014	-2.046213	-0.754873
40	1	0.095326	-1.186635	1.296863

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MP2/6-31+G(d,p) Sum of electronic and thermal free energies: -584.176561 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.072165	-1.234280	-1.254785
2	1	-3.634753	-0.545093	-1.887205
3	1	-2.451191	-1.858608	-1.901054
4	1	-3.789160	-1.878686	-0.743086
5	6	-2.216357	-0.468400	-0.249259
6	6	-1.344830	-1.406455	0.600588
7	6	-0.226528	-0.512015	1.138437
8	1	-0.558849	0.052497	2.012004
9	6	1.077928	-1.267030	1.427601
10	1	1.756047	-0.696109	2.083455
11	6	1.739136	-1.352538	0.107059
12	6	1.304172	-0.284548	-0.738287
13	6	2.578426	0.715044	-0.611800
14	1	3.143203	0.559193	0.311500
15	1	3.242371	0.551837	-1.458795
16	6	1.845706	2.052631	-0.564462
17	1	1.475455	2.308898	-1.561490
18	1	2.511114	2.850152	-0.227438
19	6	0.676008	1.806471	0.386716
20	6	0.102307	0.430382	-0.060368
21	6	-1.161654	0.419797	-0.956030
22	1	-0.923398	-0.007792	-1.935336
23	1	-1.552359	1.420539	-1.142775
24	6	2.688055	-2.403415	-0.268130
25	1	3.321839	-2.702272	0.566916
26	1	2.053399	-3.273145	-0.499156
27	1	3.268877	-2.163336	-1.155005
28	1	-0.915340	-2.183431	-0.049407
29	6	-3.123885	0.372772	0.654196
30	1	-3.702453	1.080605	0.058003
31	1	-2.560945	0.944777	1.393119
32	1	-3.825154	-0.268628	1.191224
33	1	-1.905578	-1.916093	1.388234
34	6	-0.303043	2.968843	0.479518
35	1	-0.672525	3.261618	-0.503104
36	1	-1.157896	2.724373	1.109867
37	1	0.194405	3.834197	0.918264
38	1	1.224866	-0.526248	-1.799882
39	1	0.973105	-2.249168	1.897028
40	1	1.105271	1.656367	1.388142

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -585.787528 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.820514	-0.494252	0.473314
2	1	-4.317291	-1.208711	-0.190942
3	1	-3.587708	-1.008455	1.411755
4	1	-4.532244	0.308316	0.691593
5	6	-2.557196	0.058905	-0.182888
6	6	-1.777582	0.980041	0.779195
7	6	-0.387703	1.050737	0.137738
8	6	0.734913	1.520274	1.168651
9	1	0.592865	2.570150	1.426011
10	6	1.936452	1.234429	0.409402
11	6	2.263439	-0.177161	0.279199
12	6	2.841686	-0.795410	-1.013420
13	1	2.609560	-0.198713	-1.899803
14	1	3.904881	-1.035393	-1.014892
15	6	1.852834	-1.971717	-0.809248
16	6	1.017417	-1.142202	0.203334
17	6	-1.517251	-1.047234	-0.470648
18	1	-1.568498	-1.789647	0.331000
19	1	-1.725748	-1.570993	-1.408533
20	6	2.639790	2.263077	-0.365539
21	1	3.664777	1.968259	-0.603465
22	1	2.105038	2.320754	-1.331793
23	1	2.586466	3.251737	0.092643
24	1	-2.240731	1.963726	0.904416
25	6	-2.930135	0.800129	-1.473652
26	1	-3.498659	0.139722	-2.135385
27	1	-2.052123	1.141675	-2.033384
28	1	-3.554007	1.673152	-1.256535
29	1	2.870757	-0.428484	1.167268
30	1	0.650072	0.872835	2.046066
31	6	-0.131074	-0.356436	-0.484426
32	1	0.186336	-0.202798	-1.525305
33	6	0.630203	-1.872799	1.483247
34	1	0.078021	-2.785954	1.245134
35	1	1.522607	-2.173788	2.039578
36	1	-0.002006	-1.272217	2.146224
37	1	2.336707	-2.821324	-0.320264
38	1	1.319254	-2.322563	-1.695802
39	1	-1.714982	0.503204	1.766739
40	1	-0.405025	1.803231	-0.657874

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -585.738908 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.945162	-0.174499	-0.636674
2	1	-4.528378	0.687243	-0.296324
3	1	-3.823123	-0.098974	-1.722093
4	1	-4.528307	-1.075495	-0.424256
5	6	-2.592792	-0.237156	0.069360
6	6	-1.706933	-1.365575	-0.456509
7	6	-0.262555	-1.019120	-0.061234
8	6	0.758242	-1.774765	-0.941039
9	1	0.473509	-2.832913	-0.918576
10	6	2.090263	-1.484275	-0.324457
11	6	2.657534	-0.345032	-0.725713
12	6	3.238014	0.655084	0.213213
13	1	3.338169	0.249685	1.222493
14	1	4.203873	1.082407	-0.074692
15	6	2.212056	1.797786	0.177820
16	6	0.707348	1.653578	0.013101
17	6	-1.726493	0.982451	-0.261087
18	1	-1.797285	1.206120	-1.335803
19	1	-2.056785	1.869217	0.282168
20	6	2.489023	-2.273248	0.890494
21	1	3.403204	-1.895605	1.350577
22	1	1.702428	-2.313631	1.653083
23	1	2.682240	-3.308389	0.588124
24	1	-1.991298	-2.348607	-0.068345
25	6	-2.800794	-0.348447	1.584755
26	1	-3.387913	0.496991	1.957541
27	1	-1.856691	-0.371470	2.143230
28	1	-3.343644	-1.265873	1.829762
29	1	2.326479	0.070365	-1.680881
30	1	0.698223	-1.425512	-1.977247
31	6	-0.262493	0.574535	0.019731
32	1	-0.026538	0.852569	1.149683
33	6	0.108860	3.041710	-0.073066
34	1	-0.582267	3.233724	0.751603
35	1	0.880005	3.809451	-0.051902
36	1	-0.467030	3.133211	-0.999554
37	1	2.425795	2.397362	-0.723811
38	1	2.354650	2.517651	0.996523
39	1	-1.779879	-1.408909	-1.551636
40	1	-0.104146	-1.358785	0.968169

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B3LYP/6-31+G(d,p) Sum of electronic and thermal free energies: -585.815456 H

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.058874	-1.241935	-1.294106
2	1	-3.618418	-0.545290	-1.926570
3	1	-2.436362	-1.865003	-1.945585
4	1	-3.783460	-1.891406	-0.792820
5	6	-2.208995	-0.486201	-0.273542
6	6	-1.348552	-1.437406	0.577822
7	6	-0.229837	-0.551127	1.133004
8	1	-0.566803	0.002774	2.014330
9	6	1.072406	-1.311058	1.424113
10	1	1.745764	-0.731018	2.088061
11	6	1.786172	-1.343121	0.138384
12	6	1.353058	-0.258611	-0.718815
13	6	2.535618	0.817387	-0.730588
14	1	3.197952	0.696668	0.134864
15	1	3.134296	0.714137	-1.636297
16	6	1.747103	2.119782	-0.605368
17	1	1.291629	2.378689	-1.569671
18	1	2.388809	2.950204	-0.297263
19	6	0.656813	1.792871	0.416540
20	6	0.112937	0.411085	-0.045704
21	6	-1.140142	0.404025	-0.961340
22	1	-0.889946	-0.022295	-1.940521
23	1	-1.528498	1.407473	-1.154630
24	6	2.792159	-2.341378	-0.220327
25	1	3.358826	-2.694396	0.645406
26	1	2.201575	-3.208227	-0.570732
27	1	3.439550	-2.029428	-1.041264
28	1	-0.916943	-2.213972	-0.076506
29	6	-3.126192	0.349079	0.629046
30	1	-3.676845	1.087506	0.037710
31	1	-2.574009	0.890742	1.403223
32	1	-3.857160	-0.293567	1.130044
33	1	-1.920671	-1.952447	1.356422
34	6	-0.360688	2.906667	0.625775
35	1	-0.811222	3.227608	-0.317377
36	1	-1.164283	2.598962	1.300740
37	1	0.127103	3.777933	1.070469
38	1	1.215304	-0.591945	-1.755437
39	1	0.981795	-2.297565	1.892622
40	1	1.164095	1.623507	1.381422