Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Aluminum(I) *β*-Diketiminato Complexes Activate C(sp^3)–F and C(sp^2)–F Bonds by Different Oxidative Addition Mechanisms: A DFT Study

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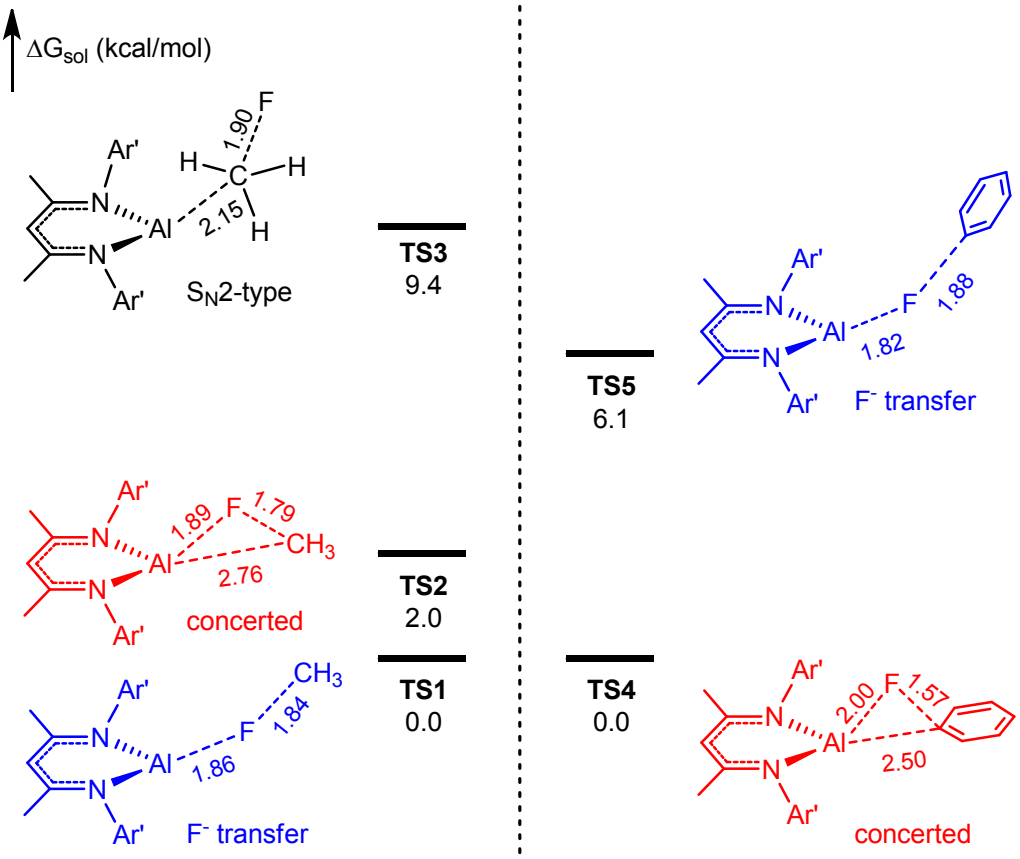

Fig. S1 TPSSh/6-311++G(d,p)–SMD//TPSSh/6-31G(d,p)-computed geometries and relative free energies of transition states for various mechanisms of oxidative additions of CH_3F (left) and C_6H_5F (right) to **1**. **TS1** is 26.7 kcal/mol relative to **1** and CH_3F; **TS4** is 32.9 kcal/mol relative to **1** and C_6H_5F. Selected bond/interatomic distances are given in Å (the same below).

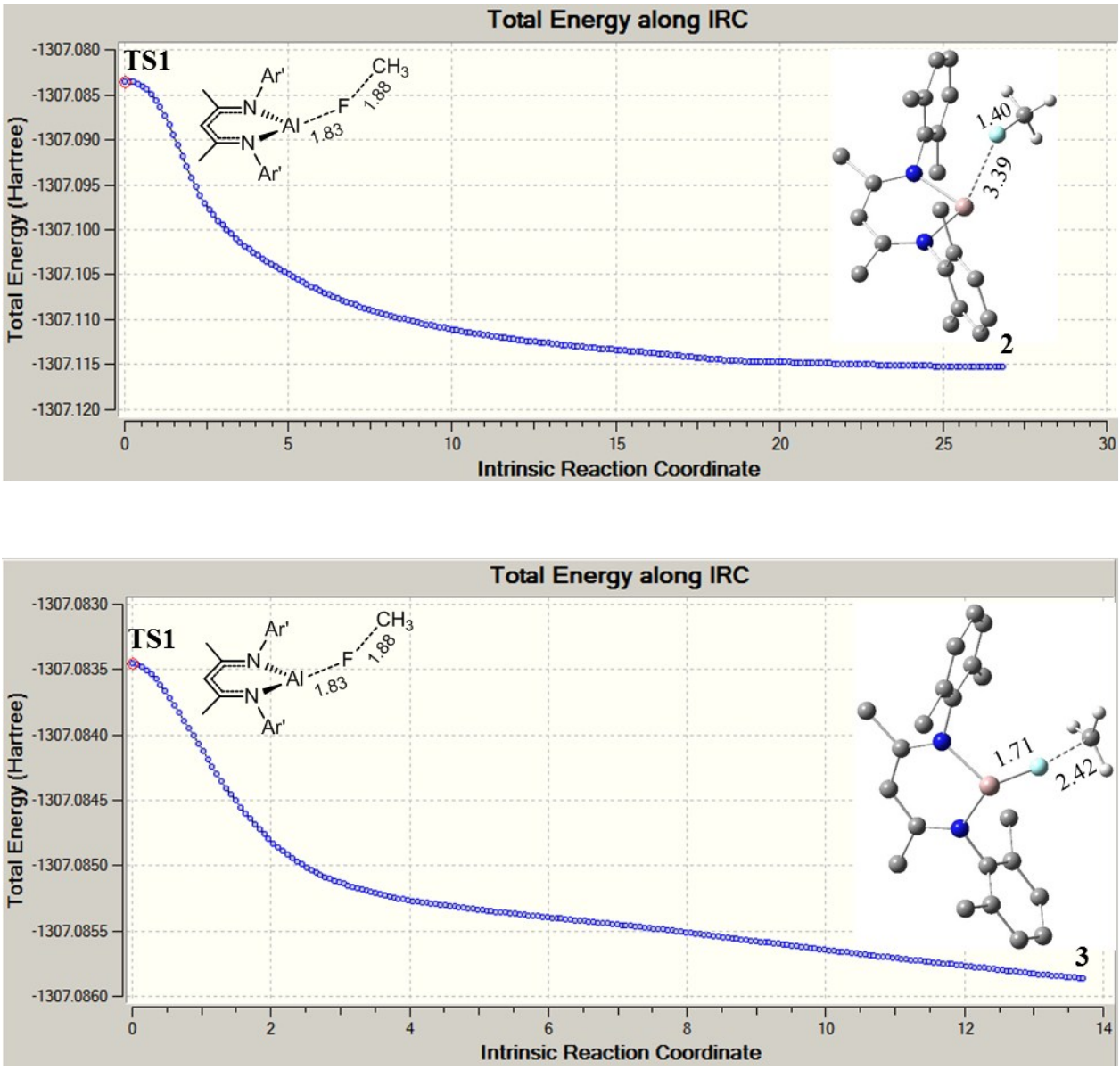

Fig. S2 B3LYP-D3/6-31G(d,p)-computed IRC plots showing the connections of **TS1**. Top, **TS1→2** (starting VDW complex); bottom, **TS1→3** (ion pair product). Hydrogen atoms of Nac'Nac' are omitted for clarity in the ball-and-stick representations (the same below).

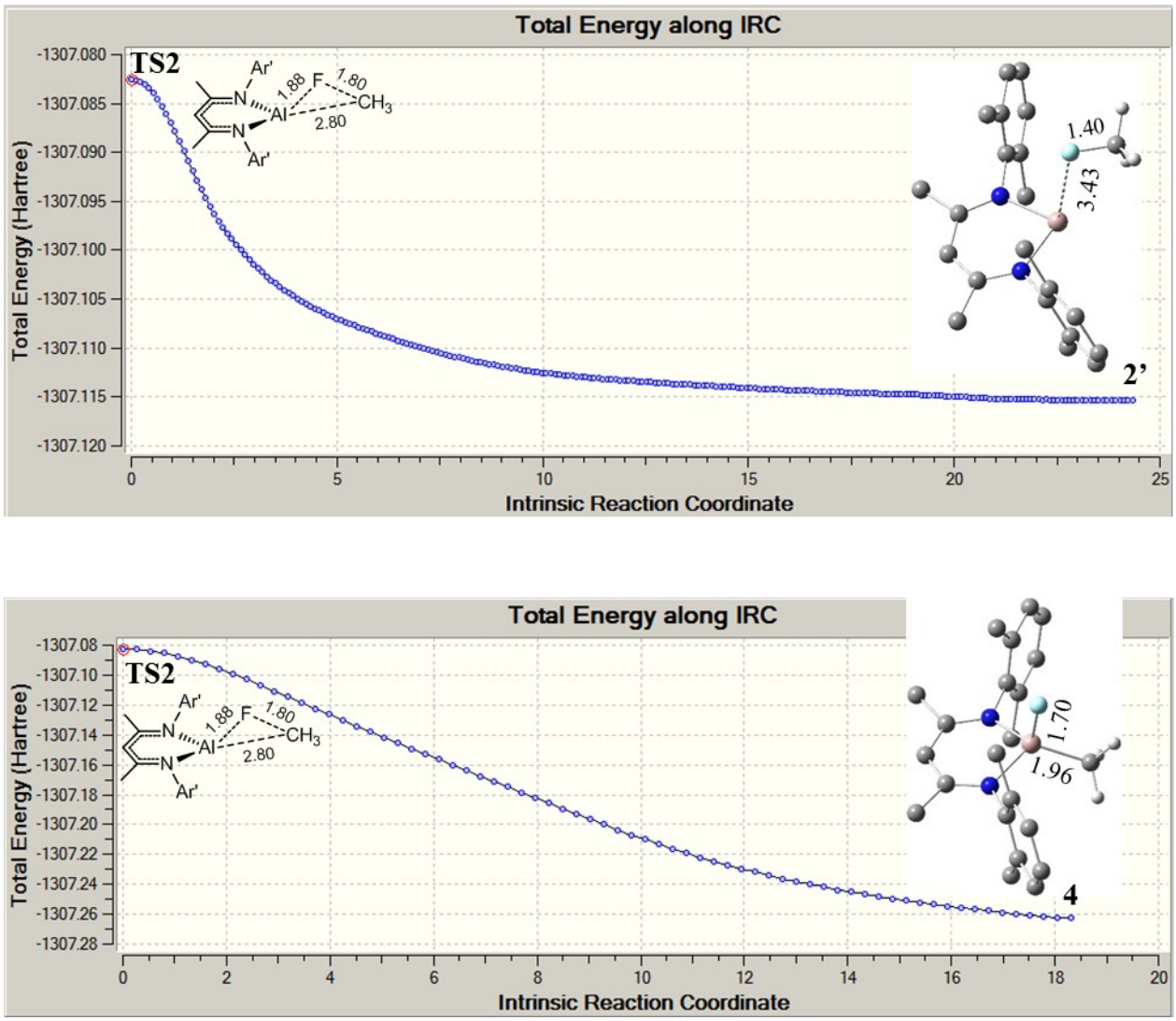

Fig. S3 B3LYP-D3/6-31G(d,p)-computed IRC plots showing the connections of **TS2**. Top, **TS2→2'** (starting VDW complex); bottom, **TS2→4** (Al^{III} complex product).

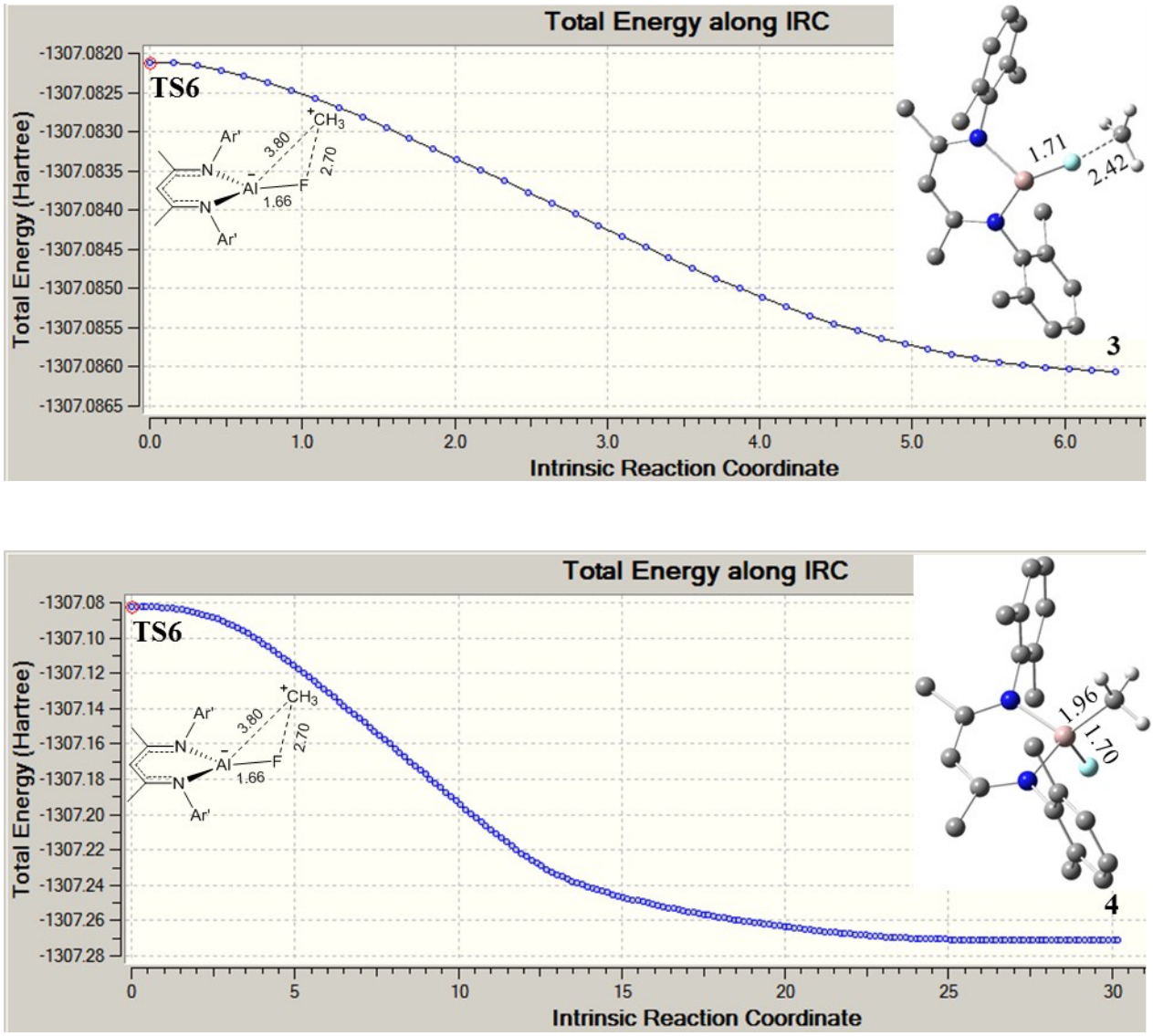

Fig. S4 B3LYP-D3/6-31G(d,p)-computed IRC plots showing the connections of **TS6**. Top, **TS6→3** (starting ion pair); bottom, **TS6→4** (Al^{III} complex product).

Cartesian Coordinates, SCF Energies, and Free Energies (298.15 K and 1 atm)

CH_3F

SCF energy: -139.73719965 a.u.

SCF energy in solution: -139.79398824 a.u.

Free energy in solution: -139.77615724 a.u.

C	0.000000	0.000000	-0.630126
H	0.000000	1.032132	-1.001080
H	-0.893853	-0.516066	-1.001080
H	0.893853	-0.516066	-1.001080
F	0.000000	0.000000	0.753777

$C_5H_{11}F$

SCF energy: -297.01919876 a.u.

SCF energy in solution: -297.11415782 a.u.

Free energy in solution: -296.99171782 a.u.

C	1.922929	0.517689	0.000223
H	1.927676	1.162482	-0.889412
H	1.928332	1.161770	0.890362
C	0.714212	-0.402500	0.000328
H	0.772660	-1.054614	-0.880014
H	0.772405	-1.054354	0.880865
C	-0.610271	0.368708	0.000101
H	-0.652467	1.029066	0.878247
H	-0.652238	1.028689	-0.878323
C	-1.839847	-0.547638	0.000087
H	-1.797816	-1.206699	-0.877442
H	-1.798036	-1.206413	0.877841
C	-3.160525	0.227983	-0.000254
H	-3.239928	0.870965	-0.884390
H	-4.022390	-0.447103	-0.000279
H	-3.240189	0.871225	0.883665
F	3.093668	-0.237829	-0.000448

$C_6H_{11}F$

SCF energy: -335.13920686 a.u.

SCF energy in solution: -335.24102437 a.u.

Free energy in solution: - 335.10779737 a.u.

C	1.853099	0.000001	-0.286286
C	1.141945	1.268162	0.212690
C	-0.345857	1.262962	-0.176288
C	-1.032965	0.000000	0.329690
C	-0.345856	-1.262964	-0.176288
C	1.141945	-1.268161	0.212689
H	-0.863336	2.144733	0.216833
H	1.231227	1.324001	1.306945
H	1.629268	2.165304	-0.184986
H	1.861087	0.000001	-1.385256
H	2.900697	-0.000002	0.036470
H	-1.047803	-0.000001	1.430496
H	-0.863332	-2.144735	0.216837
H	-0.448532	-1.286827	-1.269104
H	1.231225	-1.323998	1.306945
H	1.629273	-2.165302	-0.184983
H	-0.448529	1.286826	-1.269105
F	-2.365012	0.000001	-0.102036

C_6H_5F

SCF energy: -331.49025946 a.u.

SCF energy in solution: -331.59356131 a.u.

Free energy in solution: -331.52988531 a.u.

C	1.836371	0.000004	-0.000007
C	1.135747	1.208997	0.000023
C	-0.260438	1.217681	-0.000007
C	-0.932208	-0.000025	0.000057
C	-0.260437	-1.217694	0.000046
C	1.135784	-1.208968	-0.000037
H	2.921797	0.000037	-0.000039
H	1.674874	2.151616	-0.000002
H	-0.829829	2.140636	-0.000048
H	-0.829744	-2.140698	0.000039
H	1.674884	-2.151603	-0.000065
F	-2.282321	0.000005	-0.000038

$C_6H_2F_4$

SCF energy: -629.166322423 a.u.

SCF energy in solution: -629.37863616 a.u

Free energy in solution: -629.34332216 a.u

C	1.197649	0.697396	0.000038
C	-0.000078	1.402823	0.000093
C	-1.197761	0.697463	0.000025
C	-1.197588	-0.697388	0.000082
C	0.000068	-1.402845	0.000007
C	1.197778	-0.697441	0.000060
F	-2.367651	1.354430	-0.000022

F	2.367446	1.354622	-0.000120
F	-2.367449	-1.354584	-0.000084
F	2.367584	-1.354476	0.000016
H	0.000332	2.485855	0.000130
H	-0.000118	-2.485849	-0.000067

C_6F_6

SCF energy: -827.59613629 a.u.

SCF energy in solution: -827.87944851 a.u.

Free energy in solution: -827.86294951 a.u.

C	1.234539	0.647464	-0.000198
C	1.177934	-0.745610	-0.000203
C	-0.056581	-1.393485	-0.000607
C	-1.234450	-0.647585	-0.000202
C	-1.178032	0.745496	-0.000200
C	0.056579	1.393445	-0.000098
F	-2.307179	1.458849	0.000581
F	-0.110928	-2.727998	0.000138
F	2.307233	-1.458684	0.000101
F	2.417742	1.267003	0.000591
F	-2.417783	-1.266834	0.000111
F	0.110922	2.727847	-0.000517

1

SCF energy: -1167.36508164 a.u.

SCF energy in solution: -1167.61997572 a.u.

Free energy in solution: -1167.26152372 a.u.

N	1.403780	-0.000209	0.292022
C	1.254399	-0.000453	1.624771
C	-0.000003	-0.000608	2.252515
C	-1.254404	-0.000459	1.624763
N	-1.403782	-0.000213	0.292020
H	-0.000006	-0.000810	3.335071
Al	0.000012	-0.000099	-1.156204
C	2.481381	-0.000524	2.513947
H	3.105138	0.875839	2.313378
H	2.205083	-0.000858	3.569558
H	3.105427	-0.876563	2.312886
C	-2.481391	-0.000522	2.513934
H	-3.105439	-0.876560	2.312870
H	-2.205101	-0.000855	3.569546
H	-3.105142	0.875843	2.313356
C	2.746403	0.000037	-0.234939
C	3.379951	1.227475	-0.507991
C	3.380238	-1.227153	-0.508438
C	4.672981	1.206645	-1.042360
C	4.673263	-1.205824	-1.042798
C	5.319303	0.000534	-1.306492
H	5.172432	2.148194	-1.255120
H	5.172935	-2.147179	-1.255899
H	6.322877	0.000726	-1.721959
C	-2.746400	0.000023	-0.234945
C	-3.380207	-1.227169	-0.508495
C	-3.379979	1.227458	-0.507939
C	-4.673232	-1.205848	-1.042856
C	-4.673009	1.206620	-1.042310
C	-5.319300	0.000506	-1.306499
H	-5.172882	-2.147206	-1.255996
H	-5.172484	2.148167	-1.255021
H	-6.322876	0.000693	-1.721964
C	2.671393	2.532775	-0.238164
H	1.779581	2.630847	-0.869034
H	2.328997	2.606743	0.799759
H	3.325593	3.384223	-0.442943
C	2.671998	-2.532719	-0.239066
H	2.329585	-2.607111	0.798821
H	1.780234	-2.630805	-0.870001
H	3.326418	-3.383936	-0.444104
C	-2.671461	2.532762	-0.238030
H	-2.329059	2.606672	0.799895
H	-1.779658	2.630902	-0.868902
H	-3.325689	3.384203	-0.442749
C	-2.671936	-2.532730	-0.239179
H	-1.780177	-2.630771	-0.870130
H	-2.329509	-2.607156	0.798701
H	-3.326340	-3.383954	-0.444243

2

SCF energy: -1307.11556032 a.u.

SCF energy in solution: -1307.41816650 a.u.

Free energy in solution: -1307.02571750 a.u.

N	-1.321600	-0.678602	0.204342
C	-1.134004	-1.534305	1.219767
C	0.136621	-1.877159	1.704002
C	1.370250	-1.383873	1.252724
N	1.486599	-0.548443	0.210586
H	0.167336	-2.572209	2.533391
Al	0.053899	0.186658	-1.001613
C	-2.334099	-2.170791	1.891326

H	-2.960445	-2.681670	1.153644
H	-2.025907	-2.890877	2.651242
H	-2.966932	-1.413683	2.363696
C	2.613260	-1.827631	1.996854
H	3.127545	-0.965327	2.432765
H	2.366187	-2.528185	2.796191
H	3.327505	-2.303015	1.318189
C	-2.675369	-0.317989	-0.135585
C	-3.335872	-1.000620	-1.175510
C	-3.297241	0.745106	0.551008
C	-4.630164	-0.597919	-1.524492
C	-4.592574	1.115865	0.171189
C	-5.256540	0.454591	-0.860705
H	-5.147630	-1.119680	-2.325270
H	-5.082769	1.931611	0.696602
H	-6.261252	0.755847	-1.143129
C	2.809783	-0.104307	-0.154604
C	3.322441	1.081638	0.405320
C	3.545674	-0.845198	-1.100317
C	4.597640	1.505258	0.012494
C	4.815380	-0.386615	-1.467435
C	5.341727	0.779887	-0.915538
H	5.005522	2.416986	0.441239
H	5.391960	-0.951872	-2.194987
H	6.329279	1.123736	-1.209677
C	-2.661738	-2.143274	-1.895690
H	-1.796297	-1.789777	-2.469207
H	-2.287125	-2.899356	-1.197242
H	-3.351386	-2.630649	-2.589963
C	-2.587432	1.467459	1.671910
H	-2.222612	0.775828	2.438494
H	-1.715728	2.017858	1.307733
H	-3.259833	2.180370	2.157344
C	2.970299	-2.101902	-1.707126
H	2.669605	-2.826179	-0.942187
H	2.071994	-1.877514	-2.294867
H	3.694585	-2.585532	-2.367867
C	2.513924	1.885744	1.395257
H	1.671343	2.386754	0.907060
H	2.090916	1.257321	2.185595
H	3.132793	2.654152	1.866849
C	-1.061442	3.778299	-0.860096
H	-0.717597	3.255081	-1.755538
H	-0.914267	4.858960	-0.954141
H	-2.118390	3.551672	-0.687940
F	-0.321912	3.322059	0.238881

2'

SCF energy: -1307.11574759 a.u.

SCF energy in solution: -1307.41807865 a.u.

Free energy in solution: -1307.02592365 a.u.

N	-1.406545	-0.584328	0.240493
C	-1.254741	-1.401675	1.292754
C	-0.000080	-1.795771	1.780168
C	1.254591	-1.401784	1.292693
N	1.406418	-0.584418	0.240453
H	-0.000089	-2.464261	2.631618
Al	-0.000057	0.230307	-0.954290
C	-2.479510	-1.939918	2.004526
H	-3.129862	-2.475023	1.305958
H	-2.199986	-2.616307	2.813911
H	-3.077564	-1.123485	2.420558
C	2.479360	-1.940072	2.004430
H	3.077500	-1.123664	2.420389
H	2.199834	-2.616406	2.813861
H	3.129630	-2.475254	1.305844
C	-2.749800	-0.232050	-0.150570
C	-3.405872	-1.004181	-1.129086
C	-3.364682	0.898068	0.423329
C	-4.695266	-0.629851	-1.523029
C	-4.656248	1.237056	0.003106
C	-5.319467	0.482955	-0.962879
H	-5.210318	-1.220131	-2.276450
H	-5.142608	2.104607	0.441560
H	-6.321130	0.761312	-1.277855
C	2.749690	-0.232179	-0.150582
C	3.364629	0.897866	0.423404
C	3.405748	-1.004301	-1.129115
C	4.656217	1.236813	0.003220
C	4.695170	-0.630017	-1.523012
C	5.319414	0.482732	-0.962798
H	5.142618	2.104311	0.441735
H	5.210213	-1.220293	-2.276442
H	6.321099	0.761052	-1.277736
C	-2.729982	-2.209401	-1.737137
H	-1.839755	-1.916158	-2.306597
H	-2.392271	-2.916647	-0.971776
H	-3.405973	-2.737468	-2.414799
C	-2.649405	1.727068	1.462944
H	-2.237488	1.108348	2.266883
H	-1.807360	2.276075	1.030012
H	-3.330340	2.455134	1.912770

C	2.729832	-2.209485	-1.737210
H	2.392059	-2.916726	-0.971872
H	1.839642	-1.916193	-2.306703
H	3.405828	-2.737571	-2.414853
C	2.649389	1.726822	1.463079
H	1.807292	2.275808	1.030221
H	2.237550	1.108072	2.267034
H	3.330329	2.454901	1.912877
C	0.000795	4.069535	-0.923259
H	0.000161	3.312074	-1.711619
H	0.898394	4.692321	-0.991694
H	-0.895642	4.693985	-0.991781
F	0.000129	3.420603	0.318250

3

SCF energy: -1307.08609803 a.u.

SCF energy in solution: -1307.39194785 a.u.

Free energy in solution: -1307.00269085 a.u.

N	-1.415232	-0.568165	0.234357
C	-1.257432	-1.372531	1.294487
C	-0.000005	-1.778595	1.769912
C	1.257398	-1.372561	1.294413
N	1.415163	-0.568148	0.234314
H	0.000013	-2.440851	2.625818
Al	-0.000055	0.096585	-0.899135
C	-2.482752	-1.859668	2.036007
H	-3.176557	-2.362723	1.356407
H	-2.210395	-2.547300	2.837888
H	-3.028881	-1.014972	2.467610
C	2.482777	-1.859965	2.035651
H	3.029063	-1.015417	2.467339
H	2.210477	-2.547736	2.837432
H	3.176421	-2.362952	1.355827
C	-2.745611	-0.153924	-0.143688
C	-3.469424	-0.916744	-1.078740
C	-3.268096	1.029418	0.411260
C	-4.747508	-0.478494	-1.443471
C	-4.549847	1.431820	0.019752
C	-5.286486	0.685563	-0.898565
H	-5.319216	-1.056982	-2.164208
H	-4.967818	2.343019	0.439148
H	-6.279356	1.013489	-1.192848
C	2.745541	-0.153893	-0.143717
C	3.268018	1.029466	0.411219
C	3.469412	-0.916780	-1.078663
C	4.549749	1.431898	0.019680
C	4.747479	-0.478503	-1.443421
C	5.286402	0.685625	-0.898614
H	4.967707	2.343111	0.439057
H	5.319239	-1.057057	-2.164064
H	6.279271	1.013553	-1.192898
C	-2.876186	-2.170638	-1.673112
H	-1.959293	-1.941704	-2.230745
H	-2.596691	-2.897137	-0.901756
H	-3.580217	-2.653285	-2.355726
C	-2.451083	1.843609	1.382870
H	-2.143736	1.252658	2.253385
H	-1.536552	2.203134	0.898744
H	-3.016638	2.707322	1.742064
C	2.876321	-2.170870	-1.672758
H	2.596869	-2.897199	-0.901224
H	1.959426	-1.942161	-2.230482
H	3.580426	-2.653618	-2.355225
C	2.451053	1.843594	1.382927
H	1.536314	2.202860	0.899016
H	2.144066	1.252691	2.253600
H	3.016499	2.707479	1.741875
C	0.000502	4.084938	-0.153242
H	0.932496	4.197114	-0.686201
H	0.000687	4.103842	0.928350
H	-0.931577	4.197782	-0.685912
F	-0.000241	1.806115	-0.961703

4

SCF energy: -1307.27149642 a.u.

SCF energy in solution: -1307.57364271 a.u.

Free energy in solution: -1307.17965671 a.u.

N	1.422501	-0.278211	0.424437
C	1.259003	-0.707427	1.682460
C	-0.000040	-0.961709	2.252747
C	-1.259045	-0.707388	1.682394
N	-1.422472	-0.278220	0.424351
H	-0.000070	-1.326587	3.271668
Al	0.000063	-0.159472	-0.859719
C	2.479804	-0.900176	2.554813
H	2.999368	0.051770	2.703535
H	2.208200	-1.305039	3.530480
H	3.196796	-1.573972	2.077221
C	-2.479893	-0.899891	2.554730
H	-3.196950	-1.573663	2.077204

H	-2.208370	-1.304652	3.530462
H	-2.999344	0.052144	2.703301
C	2.740041	0.076043	-0.040936
C	3.185521	1.400505	0.134226
C	3.528651	-0.886936	-0.699790
C	4.445818	1.750474	-0.361932
C	4.783542	-0.494048	-1.181342
C	5.240866	0.811900	-1.017536
H	4.801208	2.769449	-0.233330
H	5.404177	-1.225993	-1.691266
H	6.215985	1.098435	-1.400863
C	-2.740001	0.076039	-0.041065
C	-3.528706	-0.886934	-0.699839
C	-3.185458	1.400494	0.134170
C	-4.783602	-0.493990	-1.181334
C	-4.445758	1.750517	-0.361938
C	-5.240858	0.811981	-1.017531
H	-5.404307	-1.225920	-1.691195
H	-4.801126	2.769490	-0.233267
H	-6.215994	1.098547	-1.400792
C	2.320775	2.413544	0.845148
H	1.365812	2.547977	0.328714
H	2.080922	2.099245	1.867204
H	2.819573	3.384504	0.899187
C	3.038525	-2.304610	-0.874125
H	2.838682	-2.780944	0.092985
H	2.099286	-2.335350	-1.432974
H	3.781945	-2.910200	-1.398796
C	-2.320704	2.413436	0.845212
H	-2.080674	2.098904	1.867155
H	-1.365834	2.548065	0.328658
H	-2.819573	3.384344	0.899551
C	-3.038741	-2.304673	-0.874096
H	-2.099529	-2.335550	-1.432974
H	-2.838936	-2.780981	0.093035
H	-3.782246	-2.910207	-1.398713
C	0.000075	1.433344	-2.001253
H	0.000695	2.393888	-1.474524
H	-0.880475	1.430344	-2.655675
H	0.879965	1.429714	-2.656557
F	0.000100	-1.593619	-1.770411

5

SCF energy: -1498.86968454 a.u.

SCF energy in solution: -1499.21982626 a.u.

Free energy in solution: -1498.77936226 a.u.

N	0.264273	-1.615246	-0.095984
C	-0.276739	-2.486701	-0.959076
C	-1.632169	-2.460712	-1.319364
C	-2.574918	-1.490982	-0.946026
N	-2.317056	-0.533608	-0.043198
H	-1.963620	-3.216695	-2.019896
Al	-0.661351	-0.247941	1.068185
C	0.600847	-3.538376	-1.607226
H	1.162401	-4.094334	-0.850627
H	0.006206	-4.240319	-2.194406
H	1.342100	-3.074824	-2.265472
C	-3.927457	-1.530901	-1.627115
H	-4.080842	-0.622173	-2.218159
H	-4.011641	-2.395065	-2.288199
H	-4.738529	-1.563570	-0.894167
C	1.699509	-1.593239	0.034678
C	2.320076	-2.276549	1.096744
C	2.448723	-0.829111	-0.882925
C	3.710763	-2.181334	1.227442
C	3.835383	-0.761715	-0.719276
C	4.464806	-1.428132	0.330244
H	4.201314	-2.704747	2.044079
H	4.419730	-0.157773	-1.406824
H	5.541907	-1.356166	0.450585
C	-3.328273	0.467071	0.189586
C	-3.313412	1.647102	-0.579353
C	-4.278611	0.268615	1.209452
C	-4.287867	2.618923	-0.325446
C	-5.234785	1.265334	1.433090
C	-5.244301	2.432042	0.670830
H	-4.289674	3.532047	-0.914892
H	-5.975245	1.121579	2.215645
H	-5.993186	3.196690	0.856314
C	1.502855	-3.093584	2.067865
H	0.830266	-2.454655	2.652740
H	0.869568	-3.823460	1.551617
H	2.147934	-3.634300	2.765543
C	1.764670	-0.093962	-2.010688
H	1.205042	-0.772323	-2.664095
H	1.046947	0.638288	-1.630160
H	2.495246	0.441751	-2.621469
C	-4.255444	-0.988492	2.044476
H	-4.320879	-1.891836	1.428029
H	-3.319235	-1.064193	2.610451
H	-5.084758	-1.001770	2.756531

C	-2.260409	1.863716	-1.640661
H	-1.274764	2.032726	-1.191478
H	-2.161297	0.997365	-2.302607
H	-2.499327	2.736849	-2.253933
F	0.976586	2.755227	-0.513563
C	4.879263	2.351651	0.743073
C	3.830342	2.001378	1.597012
C	2.503456	2.142573	1.187422
C	2.262034	2.634891	-0.088690
C	3.281530	2.989605	-0.963374
C	4.603089	2.846618	-0.533741
H	3.032630	3.365950	-1.949597
H	5.414858	3.120872	-1.201240
H	5.908140	2.235304	1.069618
H	4.040967	1.603592	2.584849
H	1.667757	1.858992	1.817439

6

SCF energy: -1499.01661294 a.u.

SCF energy in solution: -1499.36655330 a.u.

Free energy in solution: -1498.92031530 a.u.

N	-1.490055	-1.062428	-0.022159
C	-1.378110	-2.302489	-0.523744
C	-0.147631	-2.948212	-0.723173
C	1.134381	-2.385885	-0.593545
N	1.349913	-1.170458	-0.076965
H	-0.192056	-3.956223	-1.114397
Al	-0.017891	-0.134642	0.780290
C	-2.631872	-3.037575	-0.943744
H	-3.109243	-2.531214	-1.788762
H	-2.405771	-4.063545	-1.236743
H	-3.366067	-3.051219	-0.133370
C	2.310815	-3.182263	-1.111525
H	3.086968	-3.278645	-0.347284
H	2.002630	-4.177732	-1.433709
H	2.771611	-2.667070	-1.960759
C	-2.779906	-0.418908	-0.043718
C	-3.161637	0.281695	-1.205189
C	-3.603159	-0.463593	1.097061
C	-4.394734	0.941995	-1.208177
C	-4.827053	0.216231	1.053146
C	-5.222411	0.913556	-0.086376
H	-4.699274	1.490282	-2.095602
H	-5.473314	0.193417	1.926405
H	-6.174729	1.435750	-0.100545
C	2.675672	-0.607649	-0.120144
C	3.537028	-0.774070	0.980723
C	3.043383	0.164194	-1.238758
C	4.790560	-0.150879	0.936114
C	4.306515	0.764450	-1.244707
C	5.175164	0.611789	-0.165173
H	5.466642	-0.267110	1.778868
H	4.601149	1.367916	-2.098977
H	6.150220	1.090227	-0.180411
C	-2.235717	0.360198	-2.395169
H	-1.342374	0.943353	-2.144830
H	-1.890074	-0.626447	-2.719695
H	-2.728340	0.845005	-3.241852
C	-3.186111	-1.235800	2.325881
H	-3.041248	-2.298140	2.096331
H	-2.233575	-0.878843	2.727054
H	-3.946804	-1.161404	3.107094
C	2.071721	0.386795	-2.371405
H	1.631039	-0.548575	-2.730884
H	1.245656	1.022799	-2.033556
H	2.559142	0.883436	-3.214195
C	3.119748	-1.598137	2.175690
H	2.183316	-1.233952	2.607411
H	2.946646	-2.645271	1.899581
H	3.893317	-1.580208	2.947539
F	0.006955	-0.526571	2.430750
C	0.426105	4.608530	0.062589
C	1.526502	3.826059	0.417284
C	1.374119	2.452015	0.615708
C	0.127341	1.803754	0.460465
C	-0.965818	2.629542	0.120571
C	-0.824200	4.005424	-0.079180
H	-1.957698	2.200956	0.012457
H	-1.691945	4.605323	-0.343047
H	0.540903	5.678014	-0.094468
H	2.504729	4.284393	0.540595
H	2.255355	1.879828	0.894092

TS1

SCF energy: -1307.08345410 a.u.

SCF energy in solution: -1307.38737812 a.u.

Free energy in solution: -1306.99544212 a.u.

1 imaginary frequency: -267.92 cm^{-1}

N	-1.344283	-0.758565	0.037499
C	-1.162355	-1.718319	0.953185

C	0.106916	-2.148264	1.369619
C	1.337973	-1.554316	1.039609
N	1.463302	-0.608159	0.102909
H	0.133675	-2.946432	2.100416
Al	0.053578	-0.026657	-1.180142
C	-2.370301	-2.360263	1.604395
H	-3.095432	-2.675428	0.848498
H	-2.080128	-3.226247	2.201897
H	-2.887793	-1.649953	2.256572
C	2.560744	-2.002633	1.812911
H	2.968179	-1.168951	2.394252
H	2.318931	-2.818008	2.496549
H	3.357614	-2.328554	1.138575
C	-2.652497	-0.186197	-0.111084
C	-3.485281	-0.588798	-1.172442
C	-3.053445	0.821385	0.790484
C	-4.726629	0.041212	-1.321387
C	-4.300974	1.427853	0.605999
C	-5.133836	1.044719	-0.444549
H	-5.377270	-0.262414	-2.137171
H	-4.617394	2.207636	1.294390
H	-6.098116	1.526510	-0.578376
C	2.755500	-0.010147	-0.108895
C	3.090882	1.153155	0.609108
C	3.638469	-0.568394	-1.053141
C	4.338529	1.743337	0.382717
C	4.877092	0.052571	-1.252398
C	5.229247	1.197624	-0.540382
H	4.608071	2.640810	0.933512
H	5.568070	-0.369834	-1.977214
H	6.194337	1.667064	-0.708349
C	-3.049364	-1.682733	-2.115555
H	-2.128399	-1.402620	-2.641499
H	-2.828299	-2.611855	-1.577802
H	-3.822488	-1.893236	-2.859215
C	-2.156950	1.225825	1.936703
H	-2.154970	0.474397	2.735582
H	-1.122247	1.330109	1.603615
H	-2.484091	2.172186	2.375725
C	3.252391	-1.802813	-1.830068
H	3.011843	-2.643071	-1.169036
H	2.356057	-1.614083	-2.433204
H	4.059661	-2.115247	-2.497626
C	2.104919	1.748071	1.583516
H	1.184876	2.015808	1.056949
H	1.825435	1.037553	2.369635
H	2.511328	2.643597	2.061166
C	-0.892623	3.386855	-0.299480
H	-0.555457	4.022103	-1.106743
H	-0.377306	3.476490	0.646787
H	-1.939877	3.119245	-0.274133
F	-0.212100	1.776404	-0.980884

TS2

SCF energy: -1307.08255141 a.u.

SCF energy in solution: -1307.38429839 a.u.

Free energy in solution: -1306.99233039 a.u.

1 imaginary frequency: -508.37 cm^{-1}

N	-1.409417	0.597745	-0.073735
C	-1.255632	1.744289	-0.745843
C	0.000000	2.308399	-1.023965
C	1.255632	1.744289	-0.745843
N	1.409417	0.597745	-0.073735
H	0.000000	3.251633	-1.554924
Al	0.000000	-0.461810	0.848813
C	-2.480447	2.481363	-1.248049
H	-3.177129	2.681224	-0.428434
H	-2.207090	3.427752	-1.717527
H	-3.026067	1.875103	-1.977692
C	2.480446	2.481364	-1.248049
H	3.026066	1.875104	-1.977692
H	2.207089	3.427752	-1.717527
H	3.177129	2.681224	-0.428434
C	-2.735713	0.059520	0.082060
C	-3.476075	0.362911	1.241950
C	-3.252692	-0.793484	-0.914096
C	-4.746604	-0.205412	1.390345
C	-4.527869	-1.339385	-0.727173
C	-5.271597	-1.052006	0.416008
H	-5.326343	0.022895	2.280938
H	-4.937229	-1.996923	-1.489836
H	-6.259359	-1.485178	0.546070
C	2.735713	0.059520	0.082059
C	3.252692	-0.793483	-0.914096
C	3.476075	0.362912	1.241950
C	4.527869	-1.339384	-0.727174
C	4.746604	-0.205412	1.390344
C	5.271596	-1.052005	0.416007
H	4.937229	-1.996922	-1.489836
H	5.326342	0.022895	2.280938
H	6.259359	-1.485177	0.546069

C	-2.910393	1.283348	2.295253
H	-2.003244	0.854540	2.738386
H	-2.623009	2.253216	1.874263
H	-3.636101	1.459492	3.093829
C	-2.448404	-1.110672	-2.151830
H	-2.165201	-0.203453	-2.697004
H	-1.518287	-1.619703	-1.885038
H	-3.017369	-1.749139	-2.833130
C	2.910393	1.283348	2.295253
H	2.623009	2.253216	1.874263
H	2.003244	0.854540	2.738386
H	3.636101	1.459492	3.093829
C	2.448404	-1.110672	-2.151831
H	1.518287	-1.619702	-1.885038
H	2.165201	-0.203452	-2.697004
H	3.017369	-1.749138	-2.833131
C	0.000003	-3.260763	1.002129
H	0.914714	-3.153647	1.567585
H	0.000003	-3.992939	0.202538
H	-0.914707	-3.153649	1.567587
F	0.000000	-1.978607	-0.258575

TS3

SCF energy: -1307.05755174 a.u.

SCF energy in solution: -1307.38054202 a.u.

Free energy in solution: -1306.98481202 a.u.

1 imaginary frequency: -497.30 cm^{-1}

N	-1.399416	-0.744374	0.123137
C	-1.252765	-1.554644	1.181630
C	0.000000	-2.010404	1.623316
C	1.252765	-1.554644	1.181630
N	1.399416	-0.744374	0.123137
H	0.000000	-2.688475	2.467001
Al	0.000000	-0.199404	-1.105758
C	-2.475697	-1.957414	1.972882
H	-3.268757	-2.321619	1.313880
H	-2.234332	-2.728485	2.706079
H	-2.882051	-1.088925	2.501706
C	2.475697	-1.957414	1.972882
H	2.882051	-1.088925	2.501706
H	2.234332	-2.728485	2.706079
H	3.268757	-2.321619	1.313880
C	-2.689216	-0.148748	-0.140642
C	-3.530229	-0.752016	-1.098093
C	-3.051581	1.046719	0.515356
C	-4.749821	-0.138288	-1.397984
C	-4.284068	1.625557	0.180683
C	-5.124564	1.046573	-0.765703
H	-5.407229	-0.595596	-2.132527
H	-4.578254	2.547359	0.675298
H	-6.073762	1.515378	-1.008747
C	2.689216	-0.148748	-0.140642
C	3.051581	1.046719	0.515356
C	3.530229	-0.752016	-1.098093
C	4.284068	1.625557	0.180683
C	4.749821	-0.138288	-1.397984
C	5.124564	1.046573	-0.765703
H	4.578254	2.547359	0.675298
H	5.407229	-0.595596	-2.132527
H	6.073762	1.515378	-1.008747
C	-3.120909	-2.034540	-1.782154
H	-2.239778	-1.882818	-2.418445
H	-2.855606	-2.815212	-1.060978
H	-3.927061	-2.414796	-2.414591
C	-2.165591	1.725000	1.536677
H	-1.497844	1.020272	2.039670
H	-1.536051	2.503348	1.078513
H	-2.778504	2.208215	2.303880
C	3.120909	-2.034540	-1.782154
H	2.855606	-2.815212	-1.060978
H	2.239778	-1.882818	-2.418445
H	3.927061	-2.414796	-2.414591
C	2.165591	1.725000	1.536677
H	1.536051	2.503348	1.078513
H	1.497844	1.020272	2.039670
H	2.778504	2.208215	2.303880
C	0.000000	1.970440	-1.070747
H	0.000000	1.595207	-0.052677
H	-0.932415	2.245723	-1.537620
H	0.932415	2.245723	-1.537620
F	0.000000	3.518049	0.044125

TS4

SCF energy: -1498.83480560 a.u.

SCF energy in solution: -1499.18255350 a.u.

Free energy in solution: -1498.74310450 a.u.

1 imaginary frequency: -384.83 cm^{-1}

N	1.412580	-1.258974	-0.000259
C	1.257197	-2.521746	-0.414918
C	-0.000026	-3.125410	-0.583416

C	-1.257238	-2.521724	-0.414921
N	-1.412601	-1.258947	-0.000265
H	-0.000034	-4.158527	-0.906354
Al	0.000003	-0.025976	0.631179
C	2.484730	-3.354725	-0.719216
H	3.156167	-3.381234	0.144571
H	2.213027	-4.376967	-0.987014
H	3.056344	-2.917286	-1.543446
C	-2.484784	-3.354686	-0.719212
H	-3.056408	-2.917232	-1.543426
H	-2.213094	-4.376927	-0.987029
H	-3.156207	-3.381202	0.144586
C	2.737910	-0.701258	0.092622
C	3.408641	-0.730498	1.332207
C	3.317390	-0.088063	-1.037769
C	4.663904	-0.119907	1.429222
C	4.575793	0.510559	-0.896340
C	5.244469	0.502578	0.326304
H	5.186170	-0.135142	2.382090
H	5.032543	0.985675	-1.760649
H	6.218494	0.974708	0.417026
C	-2.737927	-0.701222	0.092626
C	-3.317412	-0.088028	-1.037763
C	-3.408649	-0.730457	1.332215
C	-4.575813	0.510599	-0.896327
C	-4.663910	-0.119861	1.429237
C	-5.244480	0.502623	0.326321
H	-5.032566	0.985715	-1.760634
H	-5.186171	-0.135093	2.382108
H	-6.218503	0.974758	0.417049
C	2.783744	-1.405476	2.528645
H	1.860231	-0.893169	2.825997
H	2.510306	-2.444117	2.312239
H	3.467047	-1.402860	3.381849
C	2.607659	-0.063924	-2.370782
H	2.225317	-1.050632	-2.649852
H	1.745187	0.606636	-2.342181
H	3.282633	0.274263	-3.161458
C	-2.783748	-1.405433	2.528652
H	-2.510309	-2.444074	2.312246
H	-1.860235	-0.893124	2.826001
H	-3.467048	-1.402816	3.381858
C	-2.607696	-0.063914	-2.370784
H	-1.745130	0.606522	-2.342160
H	-2.225498	-1.050663	-2.649910
H	-3.282634	0.274406	-3.161432
F	0.000046	1.080972	-1.027238
C	0.000041	5.082655	0.335696
C	-1.207817	4.388307	0.200162
C	-1.224725	3.017279	-0.047461
C	0.000033	2.338811	-0.075858
C	1.224798	3.017266	-0.047422
C	1.207896	4.388294	0.200200
H	2.157306	2.474402	-0.153732
H	2.153180	4.918594	0.280236
H	0.000044	6.150892	0.527013
H	-2.153097	4.918617	0.280168
H	-2.157236	2.474426	-0.153801

TS5

SCF energy: -1498.82265073 a.u.

SCF energy in solution: -1499.17407637 a.u.

Free energy in solution: -1498.73535937 a.u.

1 imaginary frequency: -171.20 cm^{-1}

N	-1.402878	-1.427423	0.075729
C	-1.253652	-2.380546	1.004299
C	0.000003	-2.902957	1.366911
C	1.253677	-2.380590	1.004284
N	1.402913	-1.427493	0.075700
H	-0.000008	-3.706387	2.092316
Al	0.000001	-0.895417	-1.195174
C	-2.475473	-2.909899	1.723678
H	-3.247020	-3.210635	1.008900
H	-2.222056	-3.762847	2.355272
H	-2.919864	-2.132487	2.353115
C	2.475483	-2.909949	1.723684
H	2.919869	-2.132541	2.353128
H	2.222050	-3.762892	2.355276
H	3.247039	-3.210692	1.008918
C	-2.687157	-0.798041	-0.085690
C	-3.560403	-1.231055	-1.101023
C	-3.019065	0.281403	0.757107
C	-4.776534	-0.556439	-1.264699
C	-4.244148	0.928307	0.560734
C	-5.118199	0.516838	-0.445056
H	-5.458131	-0.880833	-2.046399
H	-4.509390	1.762735	1.204865
H	-6.064196	1.031150	-0.587854
C	2.687182	-0.798086	-0.085685
C	3.019009	0.281372	0.757120
C	3.560459	-1.231038	-1.101014

C	4.244039	0.928376	0.560753
C	4.776544	-0.556337	-1.264676
C	5.118124	0.516969	-0.445033
H	4.509212	1.762822	1.204889
H	5.458170	-0.880677	-2.046374
H	6.064083	1.031351	-0.587830
C	-3.193384	-2.395184	-1.987517
H	-2.294464	-2.170252	-2.575621
H	-2.962403	-3.292360	-1.402385
H	-4.005865	-2.635958	-2.677998
C	-2.065635	0.734372	1.835245
H	-1.853387	-0.060623	2.558556
H	-1.108834	1.032079	1.399811
H	-2.469243	1.591375	2.379812
C	3.193497	-2.395165	-1.987532
H	2.962606	-3.292380	-1.402421
H	2.294536	-2.170273	-2.575588
H	4.005966	-2.635856	-2.678055
C	2.065524	0.734231	1.835252
H	1.108721	1.031890	1.399794
H	1.853276	-0.060833	2.558489
H	2.469059	1.591218	2.379894
F	0.000038	0.884994	-1.286155
C	-1.224466	3.262649	-0.333075
C	-1.213969	4.604418	0.082193
C	-0.000001	5.267127	0.288402
C	1.213977	4.604386	0.082351
C	1.224493	3.262618	-0.332919
C	0.000016	2.656754	-0.494947
H	2.157184	2.728894	-0.493138
H	2.155201	5.126578	0.240527
H	-0.000008	6.305544	0.607018
H	-2.155201	5.126634	0.240246
H	-2.157151	2.728942	-0.493396

TS6

SCF energy: -1307.0821111 a.u.

SCF energy in solution: -1307.39268190 a.u.

Free energy in solution: -1307.00423190 a.u.

1 imaginary frequency: -170.33 cm^{-1}

N	-1.417240	-0.541397	0.256038
C	-1.258275	-1.355195	1.313211
C	0.000041	-1.764989	1.781906
C	1.258319	-1.355177	1.313149
N	1.417247	-0.541321	0.255996
H	0.000069	-2.434934	2.631704
Al	-0.000035	0.050046	-0.849370
C	-2.484506	-1.850167	2.043837
H	-3.177586	-2.337688	1.352179
H	-2.215088	-2.552841	2.833370
H	-3.028191	-1.011320	2.488885
C	2.484589	-1.850206	2.043675
H	3.028316	-1.011401	2.488749
H	2.215204	-2.552929	2.833176
H	3.177618	-2.337694	1.351943
C	-2.748271	-0.115856	-0.122371
C	-3.460824	-0.856130	-1.082843
C	-3.275413	1.046951	0.469272
C	-4.737370	-0.411441	-1.444300
C	-4.556234	1.454868	0.078318
C	-5.282453	0.734867	-0.868452
H	-5.302092	-0.969847	-2.185834
H	-4.980738	2.351241	0.521769
H	-6.273793	1.069202	-1.160515
C	2.748286	-0.115835	-0.122463
C	3.275602	1.046833	0.469306
C	3.460720	-0.856079	-1.083052
C	4.556445	1.454659	0.078325
C	4.737289	-0.411480	-1.444533
C	5.282528	0.734701	-0.868580
H	4.981076	2.350925	0.521871
H	5.301914	-0.969865	-2.186158
H	6.273889	1.068963	-1.160657
C	-2.862750	-2.094587	-1.704614
H	-1.933458	-1.856919	-2.239895
H	-2.601323	-2.846187	-0.950776
H	-3.556012	-2.552287	-2.414588
C	-2.470977	1.833867	1.470485
H	-2.155023	1.216837	2.319685
H	-1.555473	2.233700	1.006101
H	-3.050280	2.674532	1.860656
C	2.862509	-2.094431	-1.704899
H	2.601034	-2.846057	-0.951105
H	1.933220	-1.856636	-2.240134
H	3.555705	-2.552145	-2.414928
C	2.471329	1.833718	1.470670
H	1.555885	2.233771	1.006356
H	2.155280	1.216609	2.319775
H	3.050782	2.674225	1.860959
C	0.000376	3.765994	-0.038408
H	0.916974	3.934090	-0.592735

H	0.000389	4.103035	0.996415
H	-0.916174	3.934246	-0.592758
F	-0.000832	1.545166	-1.570198

TS (F^- transfer) for $C_5H_{11}F$

SCF energy: -1464.36718814 a.u.

SCF energy in solution: -1464.70919175 a.u.

Free energy in solution: -1464.21246775 a.u.

1 imaginary frequency: -118.55 cm^{-1}

N	0.513010	-2.021922	0.075618
C	-0.065306	-2.997719	-0.635155
C	-1.428167	-2.997292	-0.970395
C	-2.332768	-1.936575	-0.782717
N	-2.046827	-0.855219	-0.051076
H	-1.790006	-3.849322	-1.531605
Al	-0.450040	-0.621215	1.118746
C	0.781570	-4.148464	-1.138847
H	1.387185	-4.565548	-0.328897
H	0.159013	-4.939618	-1.560463
H	1.480761	-3.812674	-1.910931
C	-3.673919	-2.029993	-1.480516
H	-3.768127	-1.231929	-2.224519
H	-3.791293	-2.990593	-1.984713
H	-4.499031	-1.895151	-0.775880
C	1.945794	-1.946784	0.106452
C	2.657482	-2.415468	1.227156
C	2.611125	-1.341925	-0.980261
C	4.048924	-2.261752	1.245509
C	4.002609	-1.205526	-0.922573
C	4.720218	-1.658951	0.183489
H	4.607241	-2.620710	2.106115
H	4.523220	-0.736522	-1.753886
H	5.799790	-1.543366	0.217011
C	-3.014758	0.206788	0.026568
C	-2.933910	1.269868	-0.892295
C	-3.992320	0.188325	1.040531
C	-3.863992	2.310343	-0.796832
C	-4.904007	1.248678	1.103772
C	-4.845946	2.301492	0.192491
H	-3.811398	3.134304	-1.503921
H	-5.664173	1.244852	1.880574
H	-5.561234	3.116543	0.256691
C	1.932884	-3.076974	2.373271
H	1.210845	-2.388438	2.829364
H	1.359027	-3.947782	2.036220
H	2.634007	-3.406371	3.144618
C	1.834890	-0.860310	-2.182750
H	1.529056	-1.691901	-2.829350
H	0.920212	-0.349900	-1.875313
H	2.435020	-0.176204	-2.788846
C	-4.047343	-0.945735	2.034229
H	-4.181155	-1.915466	1.541638
H	-3.108680	-1.009949	2.597798
H	-4.868752	-0.808164	2.742301
C	-1.847273	1.282759	-1.938578
H	-0.869323	1.283096	-1.450023
H	-1.882936	0.394247	-2.579128
H	-1.923483	2.166878	-2.577284
C	1.670938	1.998753	-0.435514
H	1.183479	1.986412	-1.403386
H	2.508705	1.320978	-0.323562
F	0.413313	0.874924	0.579421
C	1.629308	3.245966	0.368221
H	0.611472	3.653720	0.371215
H	1.888899	3.020946	1.408547
C	2.603251	4.322807	-0.174443
H	3.623418	3.916310	-0.190874
H	2.347530	4.556470	-1.216904
C	2.578540	5.610019	0.660852
H	1.555498	6.008815	0.678084
H	2.829033	5.367402	1.702075
C	3.541523	6.677457	0.132590
H	3.292795	6.958367	-0.897302
H	3.508025	7.585581	0.743528
H	4.574790	6.311724	0.134527

TS (concerted) for $C_5H_{11}F$

SCF energy: -1464.36862410 a.u.

SCF energy in solution: -1464.70714368 a.u.

Free energy in solution: -1464.20806168 a.u.

1 imaginary frequency: -428.74 cm^{-1}

N	2.324232	-0.404238	0.012167
C	2.702939	-1.487509	-0.673954
C	1.859940	-2.589615	-0.902836
C	0.480521	-2.648208	-0.647616
N	-0.175439	-1.694717	0.019788
H	2.293483	-3.431548	-1.427329
Al	0.644194	-0.180967	1.071519
C	4.092870	-1.538051	-1.275394
H	4.857610	-1.330423	-0.521807

H	4.292902	-2.511681	-1.725916
H	4.201122	-0.768705	-2.047026
C	-0.286912	-3.836881	-1.189984
H	-0.973567	-3.526064	-1.984063
H	0.388635	-4.591966	-1.595708
H	-0.900573	-4.293694	-0.407803
C	3.225940	0.715413	0.084997
C	4.123539	0.816850	1.166006
C	3.165760	1.709065	-0.912125
C	4.970802	1.929407	1.227081
C	4.032379	2.803561	-0.815785
C	4.929788	2.916672	0.244572
H	5.668286	2.016595	2.056200
H	3.997285	3.574207	-1.581658
H	5.594987	3.773421	0.305782
C	-1.608907	-1.704356	0.026812
C	-2.294059	-1.105394	-1.051764
C	-2.307328	-2.219372	1.137544
C	-3.689047	-1.012878	-0.991177
C	-3.702909	-2.100006	1.162957
C	-4.392515	-1.497034	0.111852
H	-4.224502	-0.546805	-1.814640
H	-4.249738	-2.488077	2.018320
H	-5.474791	-1.410800	0.148369
C	4.169920	-0.253594	2.228721
H	3.200454	-0.340614	2.734069
H	4.389329	-1.239711	1.803697
H	4.933419	-0.028993	2.978324
C	2.174868	1.602788	-2.046157
H	2.220207	0.626395	-2.540074
H	1.155266	1.717557	-1.665686
H	2.356667	2.375150	-2.798623
C	-1.562333	-2.878654	2.271680
H	-0.962754	-3.724941	1.918096
H	-0.861455	-2.175526	2.738047
H	-2.252864	-3.244686	3.036168
C	-1.526441	-0.549574	-2.226748
H	-0.778683	0.167888	-1.880629
H	-0.986865	-1.332715	-2.770936
H	-2.196693	-0.051787	-2.933058
C	-1.697011	1.538707	1.181729
H	-2.064719	0.560064	1.466978
H	-1.242855	2.102028	1.988209
F	-0.168036	1.188133	0.129127
C	-2.455955	2.258162	0.119266
H	-1.968908	3.205328	-0.133860
H	-2.491296	1.647834	-0.786333
C	-3.907584	2.505107	0.591220
H	-4.362389	1.541251	0.854629
H	-3.911098	3.116839	1.503279
C	-4.756483	3.186252	-0.490193
H	-4.739298	2.567048	-1.397288
H	-4.296658	4.144881	-0.764608
C	-6.204670	3.413104	-0.047192
H	-6.793622	3.894900	-0.834499
H	-6.692519	2.463921	0.202461
H	-6.250236	4.051717	0.842279

TS (F^- transfer) for $C_6H_{11}F$

SCF energy: -1502.48983960 a.u.

SCF energy in solution: -1502.83891578 a.u.

Free energy in solution: -1502.33109078 a.u.

1 imaginary frequency: -61.38 cm^{-1}

C	0.030548	2.800808	-0.315422
C	1.302620	3.372692	0.204033
C	1.330397	4.895477	-0.116839
C	0.065241	5.589341	0.414256
C	-1.215886	4.928241	-0.120196
C	-1.227577	3.405305	0.201161
H	2.231515	5.345139	0.317964
H	1.336416	3.245926	1.293055
H	2.177054	2.865250	-0.212897
H	0.026840	2.429988	-1.335210
H	0.063093	5.537741	1.512036
H	0.079331	6.653203	0.148988
H	-2.106391	5.400848	0.312109
H	-1.275442	5.069494	-1.207760
H	-1.266979	3.279838	1.290140
H	-2.113719	2.920187	-0.217706
H	1.396566	5.035575	-1.204183
N	-1.427641	-1.537326	-0.066839
C	-1.280526	-2.563481	-0.910966
C	-0.029370	-3.105504	-1.251272
C	1.230933	-2.587046	-0.908071
N	1.395331	-1.562942	-0.064639
H	-0.036593	-3.957902	-1.918419
Al	-0.009992	-0.744657	1.086816
C	-2.507736	-3.173384	-1.557008
H	-3.239524	-3.469683	-0.799641
H	-2.245843	-4.046560	-2.156768
H	-3.007401	-2.444551	-2.202855

C	2.447876	-3.220369	-1.551073
H	2.958180	-2.503927	-2.202527
H	2.171551	-4.093215	-2.144821
H	3.175634	-3.523027	-0.792377
C	-2.732771	-0.959960	0.109690
C	-3.550166	-1.380058	1.176266
C	-3.145356	0.062130	-0.767923
C	-4.792018	-0.756416	1.348504
C	-4.392298	0.661257	-0.561889
C	-5.212889	0.257677	0.490677
H	-5.431216	-1.072935	2.168526
H	-4.718175	1.450858	-1.234406
H	-6.177950	0.732904	0.641887
C	2.709721	-1.006570	0.109971
C	3.139150	0.004494	-0.772412
C	3.519894	-1.434636	1.178833
C	4.395535	0.584375	-0.568805
C	4.771530	-0.830126	1.348701
C	5.209076	0.172833	0.486167
H	4.734345	1.365380	-1.244951
H	5.405198	-1.152967	2.170558
H	6.181582	0.633216	0.635576
C	-3.095852	-2.478629	2.105116
H	-2.168065	-2.194483	2.616618
H	-2.879089	-3.404934	1.560975
H	-3.856685	-2.695944	2.859500
C	-2.245474	0.494239	-1.898777
H	-2.107697	-0.300481	-2.641303
H	-1.255619	0.737987	-1.509482
H	-2.651591	1.369064	-2.414035
C	3.047932	-2.521599	2.112540
H	2.817143	-3.446943	1.572478
H	2.124392	-2.220582	2.622068
H	3.804904	-2.747127	2.868378
C	2.246180	0.446216	-1.904989
H	1.259629	0.704159	-1.516533
H	2.097973	-0.348032	-2.646008
H	2.664484	1.314367	-2.421797
F	0.008435	0.996749	0.638103

TS (concerted) for $C_6H_{11}F$

SCF energy: -1502.48961829 a.u.

SCF energy in solution: -1502.83673633 a.u.

Free energy in solution: -1502.32637333 a.u.

1 imaginary frequency: -384.68 cm^{-1}

N	1.999652	-0.885147	0.098131
C	2.242745	-2.124392	-0.337757
C	1.244538	-3.106936	-0.462992
C	-0.140176	-2.915005	-0.325043
N	-0.677968	-1.767230	0.097211
H	1.568219	-4.087944	-0.786797
Al	0.291018	-0.194461	0.880739
C	3.651464	-2.505624	-0.747014
H	4.365268	-2.286218	0.052296
H	3.716392	-3.565568	-0.998624
H	3.969431	-1.921755	-1.616937
C	-1.049971	-4.067575	-0.699985
H	-1.650514	-3.817383	-1.580357
H	-0.475639	-4.969449	-0.918787
H	-1.755952	-4.283905	0.107516
C	3.065966	0.080069	0.080074
C	3.852100	0.271056	1.233527
C	3.273166	0.851835	-1.081191
C	4.854583	1.247730	1.204571
C	4.287385	1.816044	-1.069541
C	5.073839	2.017015	0.063641
H	5.467211	1.401199	2.089237
H	4.456883	2.414570	-1.961136
H	5.856168	2.770886	0.056965
C	-2.101614	-1.594874	0.030447
C	-2.678952	-1.145296	-1.175619
C	-2.888903	-1.810159	1.179235
C	-4.057946	-0.911328	-1.210755
C	-4.263656	-1.552178	1.105647
C	-4.847884	-1.104212	-0.078013
H	-4.511389	-0.564360	-2.135932
H	-4.877994	-1.711478	1.988065
H	-5.916105	-0.910505	-0.118870
C	3.618435	-0.565990	2.466967
H	2.597966	-0.423678	2.842580
H	3.727118	-1.636212	2.256950
H	4.322868	-0.301723	3.260329
C	2.410393	0.648564	-2.303159
H	2.415341	-0.394599	-2.637572
H	1.371027	0.901209	-2.076221
H	2.754521	1.272470	-3.132749
C	-2.260257	-2.315411	2.453931
H	-1.749053	-3.271976	2.296346
H	-1.500147	-1.612524	2.816487
H	-3.011801	-2.454414	3.235853
C	-1.816518	-0.888932	-2.387492

H	-1.062513	-0.132838	-2.153255
H	-1.275579	-1.787005	-2.705077
H	-2.420188	-0.543435	-3.231386
F	-0.164031	1.014041	-0.432407
C	-2.576254	2.013570	0.222430
C	-1.169314	2.377138	0.545915
C	-0.586873	3.541817	-0.181460
C	-1.464767	4.779378	0.157457
C	-2.939226	4.509618	-0.180990
C	-3.458137	3.256658	0.539666
H	0.455930	3.703798	0.101557
H	-0.834634	2.208376	1.564854
H	-2.671516	1.771512	-0.840841
H	-2.911765	1.141624	0.786743
H	-1.369261	5.015396	1.225386
H	-1.086565	5.646955	-0.395217
H	-3.552557	5.378844	0.083906
H	-3.039476	4.369750	-1.266346
H	-3.463016	3.431140	1.623457
H	-4.491250	3.033544	0.249831
H	-0.621167	3.368486	-1.262563

TS (F^- transfer) for $C_6H_2F_4$

SCF energy: -1796.50650700 a.u.

SCF energy in solution: -1796.96659613 a.u.

Free energy in solution: -1796.55476613 a.u.

1 imaginary frequency: -384.07 cm^{-1}

N	0.051289	2.283763	-0.075633
C	0.719155	2.978029	-1.008589
C	2.020501	2.650099	-1.416244
C	2.734002	1.490207	-1.067465
N	2.318361	0.634910	-0.125395
H	2.477175	3.297789	-2.153448
Al	0.850559	0.959229	1.153391
C	0.047030	4.158853	-1.676582
H	-0.359008	4.846398	-0.928710
H	0.747786	4.700532	-2.313922
H	-0.797434	3.832404	-2.291180
C	4.015332	1.201111	-1.819579
H	3.907538	0.295217	-2.424336
H	4.280115	2.029031	-2.479133
H	4.842627	1.016206	-1.128552
C	-1.352120	2.544962	0.106615
C	-1.785217	3.379594	1.154095
C	-2.271430	1.914778	-0.756617
C	-3.161841	3.564834	1.331848
C	-3.638807	2.127835	-0.546685
C	-4.084565	2.943540	0.493159
H	-3.507593	4.205201	2.138833
H	-4.356447	1.643739	-1.204044
H	-5.148901	3.095210	0.647161
C	3.045184	-0.595377	0.062725
C	2.690156	-1.714609	-0.712686
C	4.059348	-0.666476	1.036788
C	3.374014	-2.915831	-0.499768
C	4.720511	-1.886638	1.217531
C	4.382680	-3.004704	0.457253
H	3.101715	-3.789126	-1.086008
H	5.506242	-1.955317	1.965169
H	4.902354	-3.945580	0.613932
C	-0.787193	4.061793	2.056361
H	-0.203590	3.325079	2.622758
H	-0.065429	4.654276	1.483178
H	-1.287599	4.724633	2.766897
C	-1.787120	1.023371	-1.874460
H	-1.207489	1.579349	-2.619818
H	-1.131762	0.238173	-1.489001
H	-2.626268	0.546820	-2.387226
C	4.426648	0.545056	1.858775
H	4.704462	1.396468	1.227202
H	3.578535	0.874699	2.470982
H	5.265620	0.327151	2.524659
C	1.591006	-1.616255	-1.741124
H	0.656730	-1.289754	-1.277868
H	1.827078	-0.888624	-2.526009
H	1.412998	-2.583532	-2.216858
F	-0.341720	-0.490493	1.099261
C	-2.760172	-1.381456	0.354082
C	-3.642012	-2.414322	0.043557
C	-3.171011	-3.720136	-0.116651
C	-1.819821	-4.017847	0.022261
C	-0.941400	-2.980755	0.338147
C	-1.423196	-1.698522	0.459469
H	-1.467076	-5.035541	-0.106064
H	-3.132016	-0.368754	0.473484
F	0.371177	-3.252531	0.481347
F	-4.045671	-4.695494	-0.413316
F	-4.957468	-2.172549	-0.103543

TS (concerted) for $C_6H_2F_4$

SCF energy: -1796.52075475 a.u.

SCF energy in solution: -1796.97771427 a.u.

Free energy in solution: -1796.56573727 a.u.

1 imaginary frequency: -303.75 cm^{-1}

N	2.076790	-0.931247	-0.025444
C	2.404819	-2.167569	-0.426684
C	1.475644	-3.214611	-0.535497
C	0.091487	-3.143618	-0.318179
N	-0.534621	-2.013754	0.038805
H	1.868694	-4.178848	-0.830636
Al	0.307411	-0.308513	0.567293
C	3.846475	-2.473073	-0.773037
H	4.504552	-2.255723	0.073559
H	3.970874	-3.518715	-1.058390
H	4.185164	-1.840153	-1.599129
C	-0.714023	-4.414262	-0.489326
H	-1.438742	-4.318768	-1.302888
H	-0.065835	-5.266424	-0.698993
H	-1.290911	-4.622894	0.417129
C	3.126425	0.053032	0.103335
C	3.779778	0.187303	1.344655
C	3.453786	0.876532	-0.989676
C	4.773708	1.162949	1.474305
C	4.456975	1.837630	-0.818883
C	5.112793	1.984373	0.400957
H	5.283076	1.275512	2.427675
H	4.719091	2.479108	-1.656081
H	5.887168	2.737464	0.515382
C	-1.973758	-2.009852	0.125027
C	-2.738595	-1.814841	-1.045100
C	-2.589662	-2.151083	1.384690
C	-4.131806	-1.738243	-0.922471
C	-3.984157	-2.061046	1.462082
C	-4.753102	-1.849274	0.320281
H	-4.731204	-1.585086	-1.815914
H	-4.466562	-2.161013	2.430555
H	-5.834063	-1.778198	0.396454
C	3.409904	-0.699041	2.509066
H	2.373927	-0.518747	2.822776
H	3.479085	-1.762122	2.253267
H	4.061193	-0.511976	3.366750
C	2.727581	0.756683	-2.306954
H	2.587933	-0.285275	-2.609667
H	1.731786	1.201197	-2.231077
H	3.273491	1.274230	-3.100304
C	-1.764970	-2.400688	2.624032
H	-1.092657	-3.255999	2.495397
H	-1.132162	-1.535410	2.857436
H	-2.405643	-2.595974	3.487805
C	-2.088239	-1.661548	-2.400299
H	-1.572408	-0.701061	-2.478284
H	-1.337391	-2.433681	-2.591680
H	-2.837102	-1.714597	-3.194863
F	-0.293814	0.647231	-1.228250
C	-2.253099	4.038529	0.232371
C	-2.972486	2.867039	-0.006708
C	-2.329024	1.678247	-0.315652
C	-0.924924	1.642652	-0.293352
C	-0.216672	2.846940	-0.157752
C	-0.860626	4.026383	0.166805
F	-4.317317	2.905828	0.045474
F	-2.909322	5.178638	0.520130
F	1.132298	2.805113	-0.205036
H	-2.912273	0.781098	-0.481053
H	-0.292610	4.929189	0.357351

TS (concerted) for C_6F_6

SCF energy: -1994.95853173 a.u.

SCF energy in solution: -1995.48878690 a.u.

Free energy in solution: -1995.09380090 a.u.

1 imaginary frequency: -227.01 cm^{-1}

N	1.415214	-1.831480	-0.055075
C	1.254538	-3.105562	-0.447928
C	-0.001059	-3.696186	-0.646751
C	-1.256325	-3.104723	-0.448295
N	-1.416289	-1.830548	-0.055445
H	-0.001358	-4.731010	-0.963310
Al	-0.000159	-0.557872	0.417499
C	2.475265	-3.973778	-0.665615
H	3.067993	-4.036919	0.252412
H	2.190909	-4.981762	-0.970821
H	3.131516	-3.545627	-1.428171
C	-2.477557	-3.972112	-0.666455
H	-3.133131	-3.543563	-1.429373
H	-2.193759	-4.980320	-0.971440
H	-3.070776	-4.034752	0.251288
C	2.764807	-1.352943	0.148844
C	3.322629	-1.421752	1.439887
C	3.483785	-0.815355	-0.934807
C	4.619338	-0.932782	1.632636
C	4.779059	-0.341518	-0.699969

C	5.344847	-0.394999	0.571843
H	5.059488	-0.977638	2.625186
H	5.342984	0.081234	-1.526944
H	6.350079	-0.018008	0.736230
C	-2.765652	-1.351225	0.148227
C	-3.484212	-0.813229	-0.935500
C	-3.323714	-1.419792	1.439185
C	-4.779280	-0.338742	-0.700819
C	-4.620189	-0.930147	1.631778
C	-5.345276	-0.391957	0.570906
H	-5.342879	0.084308	-1.527865
H	-5.060496	-0.974810	2.624268
H	-6.350341	-0.014459	0.735159
C	2.541302	-2.011243	2.589492
H	1.665990	-1.394324	2.829861
H	2.164653	-3.013126	2.355813
H	3.159341	-2.080389	3.488332
C	2.867516	-0.716029	-2.308631
H	2.425932	-1.662561	-2.636405
H	2.066719	0.027237	-2.313251
H	3.614729	-0.416758	-3.048110
C	-2.542891	-2.009754	2.588889
H	-2.166715	-3.011817	2.355218
H	-1.667308	-1.393294	2.829452
H	-3.161125	-2.078634	3.487615
C	-2.867754	-0.713970	-2.309243
H	-2.067607	0.030004	-2.313983
H	-2.425243	-1.660222	-2.636542
H	-3.615071	-0.415644	-3.049001
F	-0.000261	0.707433	-1.506372
C	0.001542	4.482745	0.281231
C	-1.201837	3.805557	0.077960
C	-1.199027	2.495247	-0.376006
C	0.000520	1.774367	-0.504703
C	1.200494	2.494838	-0.377710
C	1.204398	3.805165	0.076225
F	-2.370194	1.843650	-0.506779
F	-2.364500	4.437621	0.294442
F	0.002031	5.768002	0.665099
F	2.367582	4.436875	0.290921
F	2.371282	1.842935	-0.510367