

**Computational Study of the Hydrodefluorination of Fluoroarenes at
[Ru(CO)(NHC)(PR₃)₂(H)₂]: Predicted Scope and Regioselectivities.**

Supporting Information

Stuart A. Macgregor,^{*†} David McKay,[†] Julien A. Panetier^{†¶} and Michael K. Whittlesey,^{*§}

*Institute of Chemical Sciences, School of Engineering and Physical Sciences, Heriot-Watt
University, Edinburgh, EH14 4AS, UK and Department of Chemistry, University of Bath,
Claverton Down, Bath BA2 7AY, UK*

Email: s.a.macgregor@hw.ac.uk, m.k.whittlesey@bath.ac.uk.

[†] Heriot-Watt University; [§] University of Bath.

[¶]Present Address: Department of Chemistry, University of California, Berkeley, CA 94720,
USA.

Supplementary Figures (see text)

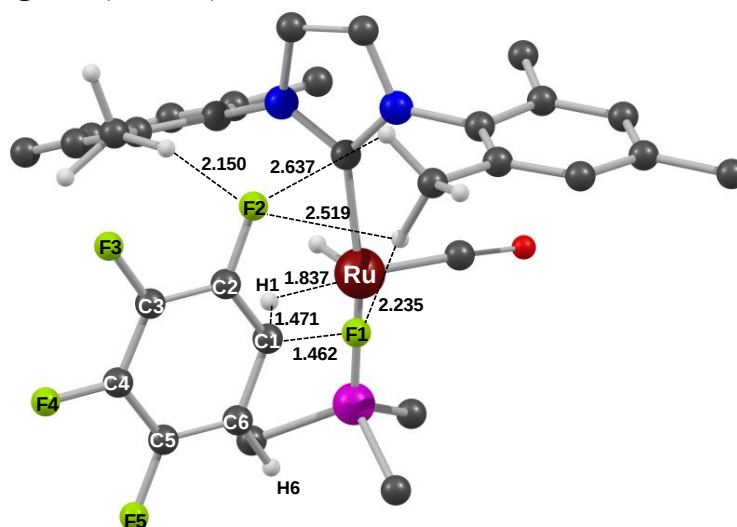


Figure S1. Computed structure of $\text{TS}(2-3)_{\text{ortho}}$ with key distances (Å). PR_3 ligands are truncated at the first substituent carbon and NHC hydrogen atoms (with the exception of those Me substituents exhibiting close contacts to F1 and F4) are omitted for clarity.

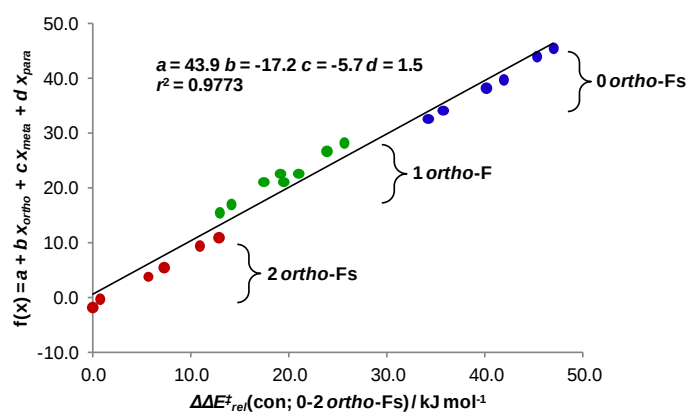


Figure S2. Plot of $f(x)$ vs. $\Delta\Delta E_{\text{rel}}^{\ddagger}(\text{con})$ (the change in computed activation barrier relative to the *para*-C–F bond of $\text{C}_6\text{F}_5\text{H}$ via the concerted pathway) where $f(x) = 43.9 \pm 1.2 + (-17.2 \pm 0.7)x_{\text{ortho}} + (-5.7 \pm 0.7)x_{\text{meta}} + (1.5 \pm 1.1)x_{\text{para}}$.

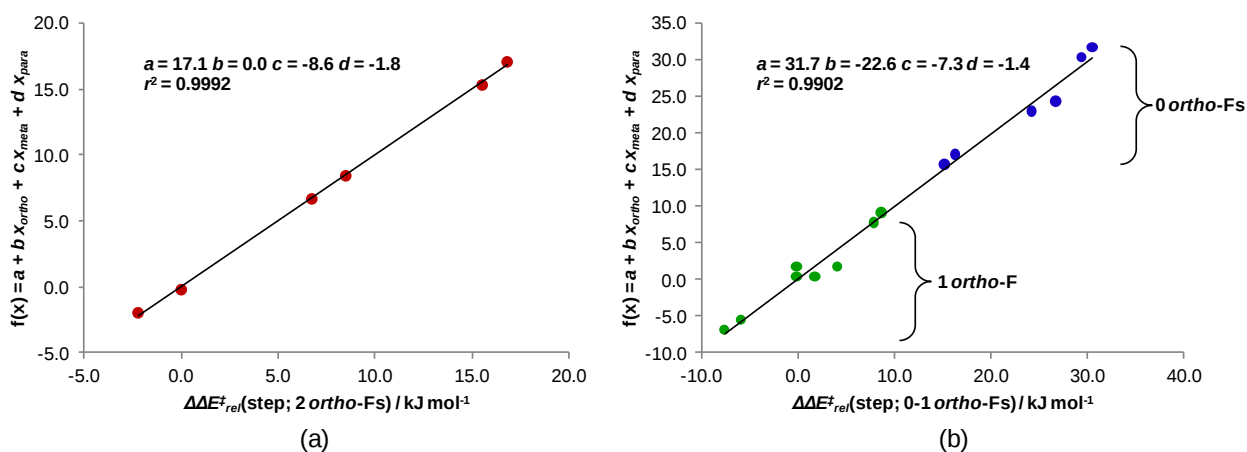


Figure S3. Plots of $f(x)$ vs. $\Delta\Delta E_{\text{rel}}^{\ddagger}(\text{step})$ (the change in computed activation barrier relative to the *para*-C–F bond of $\text{C}_6\text{F}_5\text{H}$ via the stepwise pathway) where in (a) $x_{\text{ortho}} = 2$, $f(x) = 17.1 \pm$

$0.2 + 0.0x_{ortho} + (-8.6 \pm 0.1)x_{meta} + (-1.8 \pm 0.2)x_{para}$ and in (b) $x_{ortho} < 2$, $f(x) = 31.7 \pm 0.9 + (-22.6 \pm 0.8)x_{ortho} + (-7.3 \pm 0.5)x_{meta} + (-1.4 \pm 0.8)x_{para}$.

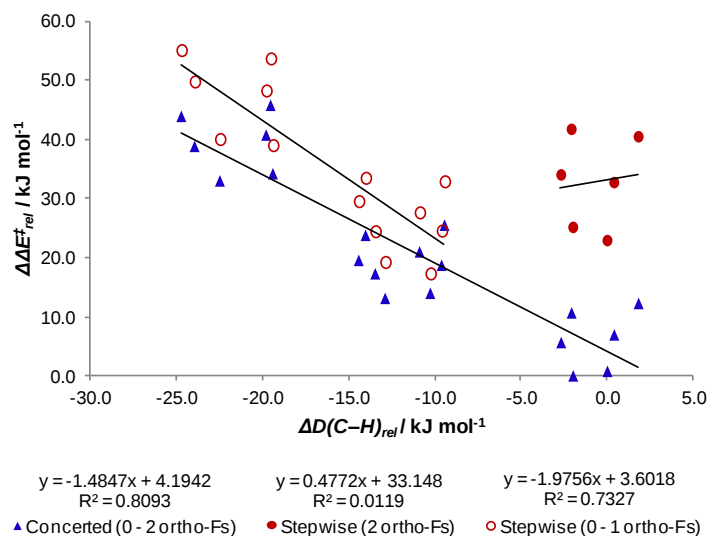


Figure S4. Plots of $\Delta\Delta E_{rel}^\ddagger$ (the change in computed activation barrier relative to the *para*-C–F bond of C_6F_5H) vs. $\Delta D(C-H)_{rel}$ (of the C–H bond formed) for $C_6F_{6-n}H_n$ ($n = 0-5$) computed with $[Ru(IME)(PMe_3)_2(CO)(H)_2]$ (Model 3).

Functional and Basis Set Testing

Functional dependency was tested by computing the barriers (based on SCF energies) for reaction of [Ru(IMes)(PPh₃)₂(CO)(H)₂] with C₆F₅H. Both the stepwise pathway via **TS(5–6)** for the *ortho*-, *meta*- and *para*- positions and the concerted pathway via **TS(2–3)**, for the lowest energy *para*-position were computed. Basis set effects were assessed via single point energy calculations on the original BP86-optimised geometries. In all cases the calculations on the stepwise pathway predict an *ortho*-regioselectivity. In addition, with only two exceptions, reaction via the stepwise pathway is preferred over the concerted route. The exceptions are for the BLYP and B3LYP functionals, where **TS(2–3)** favoured by 5.8 kJ/mol and 4.6 kJ/mol respectively. However, as the lowest form of **TS(2–3)** always corresponds to reaction at the *para*-position these functional therefore fails to model correctly the regioselectivity observed experimentally.

Table S1. Activation barriers (kJ/mol) for the stepwise and concerted pathways computed with different functionals and basis sets.

Functionals	$\Delta E^\ddagger$ (stepwise)			$\Delta E^\ddagger$ (concerted)
	<i>ortho</i>	<i>meta</i>	<i>para</i>	<i>para</i>
BP86	104.8	134.1	133.6	113.8
B3P86	125.5	162.2	162.7	134.6
BLYP	66.5	89.8	89.6	60.7
B3LYP	92.9	125.1	125.8	88.3
PBEPBE	111.3	135.2	133.7	119.2
PBE1PBE	134.5	169.7	169.8	141.3
B3PW91	116.2	154.9	155.5	121.2
M06	154.5	181.2	178.6	175.1
M06L	138.7	167.0	164.1	172.5
B97D	153.7	159.6	160.9	164.8
Basis Sets				
BP86(6-311G**)//BP86(6-31G**)	83.1	109.1	108.9	111.3
BP86(6-311++G**)//BP86(6-31G**)	88.5	112.4	114.6	126.1

Geometries
Models 1 & 2
1

SCF (BP86) Energy =	-2536.85445270		
Enthalpy 0K =	-2535.907763		
Enthalpy 298K =	-2535.843851		
Free Energy 298K =	-2536.011536		
SCRF (PCM,THF) Energy =	-2536.86615687		
Ru	0.28937	-0.08305	-0.43205
C	1.46031	1.40623	-1.26421
N	2.83378	1.39809	-1.55744
C	3.22887	2.54954	-2.25037
C	2.11511	3.31077	-2.42297
N	1.04723	2.61891	-1.83701
C	3.75148	0.27513	-1.49360
C	-0.29996	3.11055	-2.07223
H	1.96901	4.27262	-2.90685
H	4.26073	2.70231	-2.55515
C	1.64391	-1.38919	-0.11846
O	2.40224	-2.26421	0.12271
P	-1.43525	-1.73775	-0.53963
C	-1.24453	-2.92484	-2.00413
C	-1.64865	-3.00005	0.84122
C	-3.20513	-1.16385	-0.82592
H	-0.90800	1.03314	-0.70804
H	0.14814	-0.39818	-2.01429
P	0.12419	0.62570	1.88948
C	0.67798	2.35510	2.40092
C	-1.60049	0.64011	2.63562
C	1.06901	-0.37252	3.18019
C	-0.99965	2.63347	-3.21073
C	-2.26410	3.18059	-3.49424
C	-2.83156	4.20154	-2.71033
C	-2.07708	4.69691	-1.63495
C	-0.80812	4.18291	-1.30268
C	-0.41303	1.58447	-4.12246
H	-2.80702	2.81100	-4.37290
C	-4.20422	4.75881	-3.02336
H	-2.47421	5.52641	-1.03670
C	-0.04393	4.80496	-0.15904
C	4.70746	0.17903	-0.45804
C	5.62539	-0.88743	-0.49960
C	5.62448	-1.83838	-1.53208
C	4.69050	-1.68144	-2.57169
C	3.75536	-0.63354	-2.58264
C	4.77696	1.16417	0.68541
H	6.36433	-0.97090	0.30664
C	6.59212	-3.00170	-1.52328
H	4.69251	-2.39040	-3.40869
C	2.79169	-0.48571	-3.73571
C	-1.86833	0.24664	3.96389
C	-3.17903	0.29529	4.46894
C	-4.23461	0.74168	3.65650
C	-3.97368	1.14358	2.33559
C	-2.66551	1.09101	1.82794
H	-1.05254	-0.10489	4.60307
H	-3.37382	-0.01822	5.50063
H	-5.25637	0.77292	4.05027
H	-4.79016	1.48192	1.68911
H	-2.45932	1.37574	0.79082
C	1.83475	0.21494	4.21079
C	2.52578	-0.58763	5.13490
C	2.45420	-1.98649	5.05069
C	1.68918	-2.57963	4.03344
C	1.00911	-1.78070	3.10214
H	1.89369	1.30337	4.29849
H	3.11866	-0.11261	5.92450
H	2.99314	-2.61070	5.77173

H	1.62376	-3.66952	3.95281
H	0.42775	-2.25713	2.30851
C	1.88930	2.84313	1.87231
C	2.41690	4.07454	2.29058
C	1.72158	4.85607	3.22799
C	0.50086	4.39238	3.74412
C	-0.01422	3.14768	3.34162
H	2.40967	2.25088	1.11730
H	3.36608	4.42972	1.87401
H	2.12535	5.82181	3.55039
H	-0.05318	4.99648	4.47108
H	-0.95660	2.79176	3.76792
C	-3.41104	0.02955	-1.54770
C	-4.70938	0.46474	-1.85609
C	-5.82502	-0.28113	-1.44200
C	-5.63150	-1.47116	-0.72303
C	-4.33209	-1.91362	-0.42247
H	-2.54290	0.62839	-1.84263
H	-4.84257	1.39549	-2.41805
H	-6.83853	0.06217	-1.67675
H	-6.49301	-2.06236	-0.39353
H	-4.19963	-2.84500	0.13611
C	-2.35706	-3.56146	-2.59428
C	-2.18776	-4.47227	-3.64940
C	-0.90252	-4.77378	-4.12609
C	0.21167	-4.15165	-3.54243
C	0.04241	-3.22860	-2.49668
H	-3.36765	-3.33941	-2.24011
H	-3.06730	-4.94573	-4.09938
H	-0.77115	-5.48578	-4.94808
H	1.22107	-4.37774	-3.90294
H	0.91527	-2.73809	-2.06056
C	-2.39490	-2.68779	2.00051
C	-2.46410	-3.59281	3.07137
C	-1.78020	-4.81789	3.01159
C	-1.02722	-5.13281	1.86931
C	-0.96429	-4.23422	0.79141
H	-2.92732	-1.73499	2.07021
H	-3.05251	-3.33133	3.95721
H	-1.83439	-5.52180	3.84892
H	-0.49090	-6.08608	1.80800
H	-0.38207	-4.49982	-0.09603
H	1.04479	4.76288	-0.31080
H	-0.33753	5.85988	-0.03160
H	-0.25124	4.28374	0.79030
H	-4.46263	4.62621	-4.08712
H	-4.98693	4.25097	-2.42968
H	-4.26827	5.83428	-2.78676
H	0.60679	1.85475	-4.44765
H	-0.33578	0.61545	-3.59650
H	-1.03811	1.45267	-5.01989
H	4.06858	0.89095	1.48700
H	5.78613	1.17081	1.12846
H	4.53748	2.19092	0.36434
H	7.51698	-2.75657	-0.97520
H	6.14209	-3.88217	-1.02903
H	6.86895	-3.30771	-2.54614
H	1.75159	-0.62516	-3.39200
H	2.85065	0.52021	-4.18813
H	3.00638	-1.22733	-4.52132

2			
SCF (BP86) Energy =	-1835.334177		
Enthalpy 0K =	-1834.656527		
Enthalpy 298K =	-1834.608465		
Free Energy 298K =	-1834.744855		
SCRF (PCM,THF) Energy =	-1835.345737		
Ru	0.22921	0.20861	0.16085

C	1.57963	1.72689	-0.10435
N	2.95754	1.70879	-0.23674
C	3.47144	2.99227	-0.46423
C	2.40832	3.84897	-0.47453
N	1.26920	3.06748	-0.25008
C	3.79473	0.53232	-0.17403
C	-0.07860	3.58328	-0.19516
H	2.35030	4.92525	-0.61393
H	4.53645	3.16595	-0.59288
C	0.27037	0.25246	2.04893
O	0.37180	0.24660	3.22985
P	-1.33095	-1.53022	-0.02603
C	-3.04054	-0.82422	-0.31192
C	-1.16611	-2.81364	-1.38841
C	-1.58485	-2.65749	1.44918
H	0.35225	0.08541	-1.52285
H	1.40363	-0.81131	0.18532
C	-0.83627	3.63595	-1.38866
C	-2.13704	4.16524	-1.31590
C	-2.68518	4.63115	-0.10703
C	-1.89156	4.57526	1.05355
C	-0.58413	4.05720	1.03854
C	-0.26970	3.13601	-2.69819
H	-2.73781	4.21186	-2.23197
C	-4.10242	5.16023	-0.05006
H	-2.29770	4.94877	2.00154
C	0.24631	4.01041	2.30183
H	0.38066	2.97190	2.65006
H	1.25474	4.43019	2.14551
H	-0.24126	4.57881	3.10954
H	-0.96203	3.35036	-3.52701
H	0.70325	3.60645	-2.92590
H	-0.10468	2.04448	-2.65247
H	-4.44048	5.51963	-1.03579
H	-4.80437	4.36806	0.26829
H	-4.19775	5.99021	0.67015
C	4.07056	-0.16886	-1.36896
C	4.91637	-1.28996	-1.29174
C	5.48111	-1.71385	-0.07488
C	5.19114	-0.97692	1.08821
C	4.35009	0.15053	1.06743
C	3.46283	0.26286	-2.68352
H	5.13816	-1.84574	-2.21093
C	6.36136	-2.94447	-0.01383
H	5.63091	-1.28583	2.04441
C	4.04288	0.91160	2.33708
H	3.73782	1.30137	-2.94128
H	3.79819	-0.39167	-3.50369
H	2.35970	0.22332	-2.62348
H	2.99207	0.76414	2.64006
H	4.68591	0.56724	3.16250
H	4.19526	1.99762	2.21265
H	6.86735	-3.12855	-0.97598
H	7.13366	-2.85207	0.76803
H	5.76698	-3.84672	0.22096
C	-0.22428	-2.62131	-2.41691
C	-0.06632	-3.58602	-3.42712
C	-0.85236	-4.74862	-3.42336
C	-1.79700	-4.94604	-2.40163
C	-1.94923	-3.98891	-1.38769
H	0.37780	-1.70625	-2.40654
H	0.67923	-3.42829	-4.21419
H	-0.72724	-5.50219	-4.20839
H	-2.41263	-5.85200	-2.38925
H	-2.67333	-4.16385	-0.58533
C	-2.84812	-3.09525	1.89755
C	-2.94932	-3.96324	2.99829
C	-1.79198	-4.40943	3.65528

C	-0.52996	-3.98025	3.21149
C	-0.42663	-3.10571	2.11958
H	-3.75700	-2.74959	1.39430
H	-3.93712	-4.28991	3.34158
H	-1.87319	-5.08523	4.51335
H	0.37732	-4.31678	3.72458
H	0.55517	-2.75253	1.78548
C	-3.72091	-0.95380	-1.54022
C	-4.96007	-0.32017	-1.73380
C	-5.53568	0.44362	-0.70647
C	-4.85962	0.58443	0.51782
C	-3.61552	-0.03466	0.71070
H	-3.28342	-1.54397	-2.35024
H	-5.47682	-0.42981	-2.69351
H	-6.50603	0.92858	-0.85799
H	-5.30071	1.17769	1.32638
H	-3.08804	0.08550	1.66366

3

SCF (BP86) Energy =	-1934.631918		
Enthalpy 0K =	-1933.957559		
Enthalpy 298K =	-1933.909054		
Free Energy 298K =	-1934.044714		
SCRF (PCM,THF) Energy =	-1934.63987006		
Ru	0.24428	0.21299	-0.00067
C	1.84904	1.49520	-0.04840
N	3.19940	1.23354	-0.07649
C	3.94631	2.41386	-0.16387
C	3.05042	3.44646	-0.18124
N	1.77865	2.87237	-0.10499
C	3.79448	-0.08483	-0.08123
C	0.54284	3.62621	-0.11424
H	3.19259	4.52226	-0.23886
H	5.03177	2.40032	-0.21054
C	0.22844	0.30439	1.82061
O	0.30939	0.37604	3.00456
P	-1.61762	-1.33709	-0.02259
C	-2.85995	-1.23614	-1.42189
C	-1.16588	-3.15562	-0.03305
C	-2.71647	-1.17389	1.48258
H	1.20930	-0.97981	0.20143
F	0.29099	0.28991	-2.06429
C	-0.09301	3.87410	-1.35408
C	-1.28283	4.62582	-1.33409
C	-1.82898	5.13171	-0.14025
C	-1.14322	4.88839	1.06423
C	0.04703	4.13981	1.10681
C	0.47904	3.35482	-2.65228
H	-1.78961	4.82721	-2.28546
C	-3.12928	5.90689	-0.14864
H	-1.54199	5.29305	2.00238
C	0.75809	3.90052	2.42003
H	0.63470	2.85725	2.75864
H	1.84263	4.08766	2.34160
H	0.35276	4.56013	3.20363
H	-0.10088	3.73599	-3.50825
H	1.52974	3.66900	-2.78519
H	0.45679	2.24789	-2.66712
H	-3.28475	6.42607	-1.10867
H	-3.99269	5.23301	0.00216
H	-3.15825	6.65815	0.65792
C	3.90828	-0.76650	-1.31433
C	4.50989	-2.03866	-1.29938
C	4.98751	-2.62358	-0.11216
C	4.85914	-1.90144	1.08964
C	4.26080	-0.62967	1.13436
C	3.38470	-0.15327	-2.59175
H	4.61206	-2.58240	-2.24630

C	5.61052	-4.00374	-0.11927	C	-1.55702	-1.28794	-1.37796
H	5.23126	-2.33922	2.02393	C	-1.19609	-2.66689	-1.44758
C	4.11025	0.11296	2.44292	C	0.31388	-0.82687	-2.92815
H	2.28307	-0.03725	-2.54265	C	-0.13905	-3.10952	-2.21679
H	3.80418	0.85576	-2.75687	C	0.64024	-2.16455	-2.95260
H	3.64893	-0.77826	-3.45960	H	-2.59697	-1.06194	-1.13461
H	3.04777	0.19425	2.73330	F	-1.43439	0.73195	-2.72218
H	4.64438	-0.41109	3.25132	F	-1.95049	-3.56559	-0.77039
H	4.50620	1.14186	2.38265	F	1.01119	0.06636	-3.67329
H	5.90607	-4.30871	-1.13621	F	0.19791	-4.41282	-2.28178
H	6.50548	-4.04712	0.52459	F	1.70433	-2.61183	-3.65154
H	4.90214	-4.76208	0.26147	C	2.92941	-3.41279	-0.29125
C	0.01715	-3.53160	-0.70330	C	3.01151	-4.81161	-0.40068
C	0.37728	-4.88421	-0.80603	C	2.03899	-5.62788	0.19439
C	-0.43550	-5.87625	-0.23499	C	0.96761	-5.03833	0.88576
C	-1.60977	-5.50993	0.44295	C	0.87401	-3.64220	0.98470
C	-1.97577	-4.15856	0.54176	H	3.70067	-2.79079	-0.75382
H	0.65337	-2.75504	-1.14110	H	3.84258	-5.26048	-0.95529
H	1.29667	-5.16143	-1.33240	H	2.10689	-6.71760	0.11015
H	-0.15343	-6.93176	-0.31366	H	0.19398	-5.66460	1.34236
H	-2.24595	-6.27783	0.89649	H	0.02750	-3.19663	1.51633
H	-2.88466	-3.88492	1.08692	C	4.52250	-0.59031	0.48353
C	-3.90044	-0.40843	1.44092	C	5.72096	-0.14606	-0.09461
C	-4.65128	-0.19215	2.60810	C	5.69823	0.56792	-1.30492
C	-4.23099	-0.73730	3.83106	C	4.47125	0.83731	-1.92935
C	-3.05183	-1.49855	3.88317	C	3.26919	0.39777	-1.34875
C	-2.29508	-1.70956	2.72076	H	4.54963	-1.14220	1.42864
H	-4.24307	0.01327	0.49121	H	6.67368	-0.35629	0.40342
H	-5.57022	0.40176	2.55687	H	6.63434	0.91519	-1.75551
H	-4.81949	-0.57113	4.73969	H	4.44260	1.39600	-2.87084
H	-2.71236	-1.92303	4.83393	H	2.31347	0.62917	-1.82454
H	-1.37435	-2.29856	2.77627	C	2.30840	-1.81315	3.32732
C	-4.02422	-2.03555	-1.43526	C	2.63364	-1.57588	4.67546
C	-4.95267	-1.91495	-2.47843	C	2.78934	-0.26520	5.14690
C	-4.72557	-0.99958	-3.52170	C	2.61883	0.81297	4.26110
C	-3.56391	-0.21421	-3.52007	C	2.28231	0.57942	2.92051
C	-2.62775	-0.33058	-2.47734	H	2.20349	-2.84301	2.97508
H	-4.21103	-2.75026	-0.62791	H	2.76849	-2.42530	5.35388
H	-5.85366	-2.53777	-2.47865	H	3.04470	-0.08214	6.19608
H	-5.45052	-0.90927	-4.33793	H	2.74634	1.84150	4.61598
H	-3.37466	0.48864	-4.33873	H	2.14856	1.42610	2.23887
H	-1.69524	0.24456	-2.48540	C	-4.25621	0.44044	1.66298
4_{ortho}				C	-5.16950	-0.58078	1.97779
SCF (BP86) Energy =				C	-5.87542	-1.28380	0.98438
Enthalpy 0K =				C	-5.68119	-0.91115	-0.35765
Enthalpy 298K =				C	-4.77918	0.10410	-0.73034
Free Energy 298K =				C	-3.58589	1.23948	2.75815
SCRf (PCM,THF) Energy =				H	-5.33452	-0.82903	3.03286
Ru -0.36838				C	-6.81315	-2.41378	1.35090
C	-1.72686	1.74465	-0.10534	H	-6.25385	-1.41694	-1.14440
N	-1.38632	3.07949	-0.31342	C	-4.67485	0.53765	-2.17737
C	-2.51264	3.90480	-0.38016	C	0.57583	3.96361	-1.53857
C	-3.60034	3.10473	-0.20742	C	1.82522	4.60974	-1.48798
N	-3.11868	1.80232	-0.03766	C	2.43184	4.97754	-0.27425
C	-0.06522	3.67581	-0.31291	C	1.73640	4.71510	0.92011
C	-4.03372	0.73193	0.29618	C	0.48307	4.07733	0.92800
H	-4.66364	3.32677	-0.18103	C	-0.03749	3.59672	-2.86922
H	-2.42311	4.97593	-0.53849	H	2.33417	4.83648	-2.43279
C	-1.25063	-0.79455	1.50470	C	3.79675	5.63178	-0.25295
O	-1.66283	-1.37325	2.44443	H	2.17262	5.02839	1.87658
P	1.68402	-0.95195	0.61337	C	-0.25059	3.84460	2.22942
C	2.11944	-0.73852	2.43751	H	0.49615	4.09895	-3.69192
C	1.86555	-2.81176	0.41213	H	0.00632	2.50897	-3.03850
C	3.28297	-0.32348	-0.14106	H	-1.10203	3.88096	-2.92451
H	0.60940	1.19335	-0.73910	H	-1.28618	4.22535	2.18899
H	0.22748	1.15089	1.18914	H	-0.31291	2.76547	2.45772
C	-0.77075	-0.33886	-2.11466	H	0.26600	4.34555	3.06347
				H	3.91922	6.28685	0.62564

H	4.59781	4.87129	-0.20864
H	3.97081	6.23613	-1.15883
H	-5.15349	-0.20240	-2.83832
H	-5.18886	1.50345	-2.33773
H	-3.63165	0.67268	-2.49924
H	-7.60411	-2.54640	0.59444
H	-6.26551	-3.37120	1.42475
H	-7.29550	-2.23935	2.32708
H	-3.76120	0.77638	3.74113
H	-2.49865	1.31725	2.60334
H	-3.98527	2.27002	2.79038

TS (4-5)_{ortho}

SCF (BP86) Energy = -2563.697066
Enthalpy 0K = -2562.961053
Enthalpy 298K = -2562.903351
Free Energy 298K = -2563.056933
SCRF (PCM,THF) Energy = -2563.70836222
Imaginary Frequency = -560.5303 cm⁻¹

Ru	-0.32137	0.21313	0.11977
C	-1.65017	1.83172	-0.08309
N	-1.26372	3.14700	-0.33187
C	-2.35734	4.01376	-0.39702
C	-3.47095	3.26038	-0.18180
N	-3.03724	1.94516	0.00733
C	0.08060	3.68668	-0.38020
C	-3.99190	0.91088	0.34818
H	-4.52374	3.52499	-0.13458
H	-2.23028	5.07698	-0.58089
C	-0.90024	-0.27613	1.82387
O	-1.24146	-0.63942	2.89657
P	1.68859	-0.98089	0.59104
C	2.29743	-0.65995	2.34490
C	1.70499	-2.85600	0.53890
C	3.24744	-0.52977	-0.35026
H	0.19850	0.58105	-1.49215
H	0.63667	1.39502	0.62031
C	-0.73430	-0.40536	-2.12650
C	-1.60883	-1.16248	-1.24268
C	-1.47006	-2.58303	-1.17114
C	0.15875	-1.18230	-2.97170
C	-0.57375	-3.28077	-1.94987
C	0.25650	-2.54877	-2.85592
H	-2.60630	-0.77497	-1.02977
F	-1.38252	0.62134	-2.86864
F	-2.29710	-3.25822	-0.33783
F	0.95082	-0.50075	-3.84087
F	-0.43027	-4.62233	-1.87461
F	1.15007	-3.23455	-3.59641
C	2.65465	-3.61067	-0.17842
C	2.59679	-5.01528	-0.17372
C	1.59854	-5.68078	0.55209
C	0.64208	-4.93580	1.26252
C	0.68642	-3.53437	1.24735
H	3.44390	-3.10517	-0.74222
H	3.33797	-5.58727	-0.74221
H	1.55675	-6.77504	0.55546
H	-0.14982	-5.44528	1.82153
H	-0.07195	-2.96265	1.79255
C	4.51889	-0.86328	0.16932
C	5.68509	-0.53681	-0.53858
C	5.59833	0.12890	-1.77323
C	4.34021	0.46874	-2.29211
C	3.17162	0.14497	-1.58205
H	4.59691	-1.37342	1.13487
H	6.66343	-0.79997	-0.12212
H	6.50948	0.38478	-2.32469
H	4.26140	0.99087	-3.25144

H	2.19632	0.42835	-1.98438
C	2.62474	-1.69135	3.24703
C	3.10162	-1.38789	4.53481
C	3.26921	-0.05381	4.93183
C	2.95607	0.98014	4.03302
C	2.47005	0.68097	2.75236
H	2.50519	-2.73735	2.95121
H	3.34299	-2.20294	5.22571
H	3.64117	0.18103	5.93485
H	3.08628	2.02596	4.33188
H	2.21641	1.49063	2.06008
C	-4.23038	0.62459	1.71194
C	-5.16751	-0.38080	2.01678
C	-5.88647	-1.06062	1.01887
C	-5.68325	-0.68114	-0.32123
C	-4.75339	0.30938	-0.68524
C	-3.59404	1.42463	2.82747
H	-5.34411	-0.62854	3.07029
C	-6.85046	-2.17215	1.37320
H	-6.26808	-1.16604	-1.11204
C	-4.62465	0.74237	-2.13082
C	0.68801	3.93153	-1.63087
C	1.96756	4.51876	-1.63286
C	2.63026	4.87573	-0.44555
C	1.96652	4.65840	0.77654
C	0.68930	4.07437	0.83706
C	-0.00895	3.60295	-2.93061
H	2.45402	4.70850	-2.59733
C	4.02271	5.46855	-0.47865
H	2.45140	4.95977	1.71313
C	-0.00193	3.86216	2.16416
H	0.64324	3.83037	-3.78864
H	-0.29757	2.54103	-2.98123
H	-0.93835	4.18888	-3.05093
H	-1.02223	4.28439	2.16659
H	-0.09527	2.78308	2.38183
H	0.56542	4.33474	2.98145
H	4.18593	6.16764	0.35854
H	4.79051	4.67734	-0.39786
H	4.21011	6.01069	-1.42029
H	-5.21731	0.08227	-2.78361
H	-4.99815	1.77300	-2.27200
H	-3.58116	0.73079	-2.48219
H	-7.68747	-2.22686	0.65738
H	-6.34172	-3.15340	1.35663
H	-7.26942	-2.03846	2.38416
H	-3.47220	0.80908	3.73127
H	-2.60614	1.81906	2.55185
H	-4.23695	2.28608	3.08963

5_{ortho}

SCF (BP86) Energy = -2563.699150
Enthalpy 0K = -2562.960372
Enthalpy 298K = -2562.902479
Free Energy 298K = -2563.056598
SCRF (PCM,THF) Energy = -2563.71189584

Ru	-0.28189	0.26003	0.21075
C	-1.57637	1.91467	-0.00657
N	-1.15906	3.21689	-0.27428
C	-2.23067	4.10919	-0.34170
C	-3.36063	3.38499	-0.10929
N	-2.95847	2.06237	0.08957
C	0.19852	3.71534	-0.36961
C	-3.94290	1.04627	0.40110
H	-4.40628	3.67558	-0.05669
H	-2.07950	5.16662	-0.54018
C	-0.82791	-0.17485	1.89915
O	-1.16083	-0.50136	2.98921

P	1.66114	-1.05368	0.62143
C	2.37632	-0.84261	2.35044
C	1.53767	-2.91677	0.50654
C	3.18712	-0.63724	-0.38645
H	0.14341	0.46322	-1.59803
H	0.74679	1.42435	0.64891
C	-0.62683	-0.34605	-2.11826
C	-1.56070	-1.01467	-1.18500
C	-1.62255	-2.44915	-1.16160
C	0.21055	-1.24468	-2.91921
C	-0.83467	-3.24518	-1.95456
C	0.10432	-2.60900	-2.83395
H	-2.53537	-0.54221	-1.04960
F	-1.28956	0.63111	-2.97601
F	-2.54425	-3.01680	-0.34676
F	1.13560	-0.66917	-3.73354
F	-0.88272	-4.59822	-1.92776
F	0.92071	-3.40062	-3.56063
C	2.20607	-3.68831	-0.46513
C	2.01510	-5.07975	-0.52218
C	1.15998	-5.71505	0.38940
C	0.47776	-4.95109	1.35143
C	0.65542	-3.56147	1.40417
H	2.87505	-3.20732	-1.18429
H	2.53554	-5.66369	-1.28844
H	1.01322	-6.79913	0.34287
H	-0.20370	-5.43589	2.05844
H	0.10776	-2.97435	2.14940
C	4.40268	-1.32839	-0.18280
C	5.55050	-0.97830	-0.90808
C	5.50370	0.07398	-1.83888
C	4.30661	0.77863	-2.03127
C	3.15512	0.42735	-1.30648
H	4.45504	-2.13850	0.55155
H	6.48477	-1.52522	-0.74178
H	6.40114	0.34689	-2.40431
H	4.26213	1.60842	-2.74419
H	2.23313	1.00266	-1.43422
C	2.96913	-1.90976	3.05675
C	3.55557	-1.69255	4.31468
C	3.56357	-0.40836	4.87982
C	2.97988	0.65985	4.17968
C	2.38830	0.44479	2.92579
H	2.96440	-2.91831	2.63293
H	4.00498	-2.53403	4.85306
H	4.01865	-0.24130	5.86192
H	2.97720	1.66544	4.61405
H	1.92058	1.27253	2.38330
C	-4.20591	0.73511	1.75375
C	-5.17356	-0.25257	2.02148
C	-5.89574	-0.88885	0.99834
C	-5.66352	-0.48418	-0.33010
C	-4.70301	0.48828	-0.65817
C	-3.56608	1.48859	2.89954
H	-5.37121	-0.52070	3.06627
C	-6.89315	-1.98296	1.31170
H	-6.24799	-0.93679	-1.14000
C	-4.53397	0.94377	-2.09314
C	0.77309	3.92533	-1.64248
C	2.07324	4.46566	-1.68989
C	2.78428	4.81216	-0.52764
C	2.14996	4.63637	0.71680
C	0.85569	4.09992	0.82315
C	0.02090	3.62205	-2.91814
H	2.53437	4.63108	-2.67123
C	4.19616	5.35169	-0.60916
H	2.67405	4.93051	1.63422
C	0.19160	3.93585	2.17036

H	0.66068	3.80369	-3.79621
H	-0.33475	2.57953	-2.95709
H	-0.87356	4.26361	-3.01895
H	-0.79082	4.43937	2.20549
H	0.01577	2.86676	2.38610
H	0.81944	4.35710	2.97122
H	4.40143	6.07408	0.19847
H	4.93569	4.53581	-0.51222
H	4.38412	5.85205	-1.57346
H	-5.16199	0.33609	-2.76341
H	-4.83816	1.99904	-2.21646
H	-3.49054	0.86969	-2.44041
H	-7.74001	-1.97452	0.60528
H	-6.41831	-2.97852	1.23968
H	-7.29528	-1.88479	2.33341
H	-2.60107	1.93562	2.62335
H	-4.23255	2.30647	3.23257
H	-3.39469	0.82407	3.75955

TS (5-6)_{ortho}			
SCF (BP86) Energy =		-2563.689733	
Enthalpy 0K =		-2562.951364	
Enthalpy 298K =		-2562.893577	
Free Energy 298K =		-2563.048270	
SCRF (PCM,THF) Energy =		-2563.70499770	
Imaginary Frequency =		-214.7085 cm ⁻¹	
Ru	0.12582	-0.40792	0.39874
C	1.25549	-2.18119	0.11111
N	0.70097	-3.40491	-0.22758
C	1.66934	-4.40407	-0.31958
C	2.86585	-3.81988	-0.02593
N	2.60481	-2.47440	0.23626
C	-0.70049	-3.69762	-0.45607
C	3.68083	-1.55663	0.55705
H	3.87316	-4.22332	0.02579
H	1.41043	-5.42538	-0.58411
C	0.26948	-0.51250	2.19902
O	0.36262	-0.57843	3.37709
P	-1.53000	1.30697	0.66757
C	-2.36371	1.32350	2.34630
C	-0.94875	3.06715	0.47216
C	-3.04348	1.17069	-0.41905
H	0.08912	-0.57055	-1.60145
H	-1.10136	-1.38132	0.53534
C	0.66500	0.37505	-1.85536
C	1.68410	0.91181	-1.01500
C	2.12327	2.23679	-1.19723
C	0.02165	1.26385	-2.75166
C	1.55787	3.06703	-2.16199
C	0.50257	2.55622	-2.95088
H	2.32470	0.25823	-0.40848
F	1.41711	-1.09176	-2.90383
F	3.13569	2.71357	-0.43436
F	-1.02704	0.83218	-3.49703
F	1.99682	4.33008	-2.36243
F	-0.08009	3.36267	-3.86083
C	-1.49422	3.97437	-0.45759
C	-0.96310	5.27009	-0.57664
C	0.11029	5.67293	0.23173
C	0.66261	4.77216	1.15804
C	0.14486	3.47377	1.26970
H	-2.32754	3.67060	-1.09754
H	-1.38856	5.96171	-1.31112
H	0.52436	6.68156	0.13295
H	1.50941	5.07351	1.78307
H	0.59848	2.76663	1.97321
C	-4.15266	2.02298	-0.21540
C	-5.30310	1.88910	-1.00542

C	-5.36506	0.89501	-1.99768	N	0.61372	-3.27543	-0.29372
C	-4.27524	0.03399	-2.19170	C	3.61680	-1.46783	0.48894
C	-3.11890	0.16936	-1.40511	C	-0.65936	-3.50664	-0.94646
H	-4.12084	2.78355	0.57185	H	1.17944	-5.36246	-0.04556
H	-6.15533	2.55689	-0.84071	H	3.57677	-4.18612	0.80192
H	-6.26542	0.78965	-2.61221	C	1.44079	0.17302	-1.87362
H	-4.31699	-0.74784	-2.95661	O	2.14537	0.44906	-2.78342
H	-2.27955	-0.51486	-1.55274	P	-0.60261	2.01850	-0.72416
C	-2.49883	2.48628	3.12923	C	-1.61282	2.85342	0.61145
C	-3.17123	2.43451	4.36283	C	0.63122	3.35508	-1.16759
C	-3.71973	1.22741	4.82010	C	-1.81009	2.05553	-2.15993
C	-3.59288	0.06556	4.03974	H	0.03626	-1.81905	2.30746
C	-2.91624	0.11109	2.81293	H	1.51392	0.44137	0.46532
H	-2.07821	3.43429	2.78103	C	-0.84678	-0.30255	1.40397
H	-3.26557	3.34492	4.96437	C	-2.07209	-1.03292	1.39095
H	-4.24266	1.18971	5.78147	C	-2.95453	-1.03611	2.47402
H	-4.01608	-0.88167	4.39043	C	-0.61030	0.42114	2.58509
H	-2.81197	-0.79883	2.21168	C	-2.66645	-0.31013	3.64014
C	3.96978	-1.27008	1.91006	C	-1.47510	0.42572	3.69278
C	5.01259	-0.36009	2.17819	H	-2.35398	-1.63177	0.51853
C	5.77403	0.22359	1.15355	F	0.35772	-2.56484	2.81980
C	5.50577	-0.15785	-0.17562	F	-4.10458	-1.76135	2.43392
C	4.47752	-1.05676	-0.50916	F	0.51092	1.19951	2.71518
C	3.26516	-1.94671	3.06647	F	-3.50756	-0.32318	4.69594
H	5.24015	-0.11800	3.22360	F	-1.18043	1.13263	4.80495
C	6.85944	1.23204	1.46265	C	0.34905	4.38398	-2.08906
H	6.12001	0.25175	-0.98623	C	1.30510	5.37618	-2.35869
C	4.26309	-1.48510	-1.94162	C	2.54786	5.35764	-1.70555
C	-1.17789	-3.76871	-1.78666	C	2.83590	4.33609	-0.78653
C	-2.54544	-4.06447	-1.96166	C	1.88732	3.33489	-0.52421
C	-3.40902	-4.31436	-0.88083	H	-0.61462	4.40765	-2.60683
C	-2.86937	-4.30296	0.41939	H	1.07654	6.16464	-3.08380
C	-1.51609	-4.00754	0.65885	H	3.29184	6.13282	-1.91780
C	-0.27000	-3.59057	-2.98001	H	3.80569	4.30836	-0.27874
H	-2.93678	-4.11848	-2.98482	H	2.12167	2.52344	0.17256
C	-4.88010	-4.59131	-1.10689	C	-2.81844	3.03743	-2.28431
H	-3.51497	-4.54123	1.27349	C	-3.68823	3.03015	-3.38625
C	-0.96057	-4.03520	2.06486	C	-3.56762	2.04094	-4.37627
H	-0.85750	-3.63073	-3.91151	C	-2.57341	1.05727	-4.25895
H	0.30902	-2.63968	-2.96143	C	-1.70203	1.06386	-3.15776
H	0.47469	-4.40717	-3.02777	H	-2.93108	3.80336	-1.51071
H	-0.03015	-4.62632	2.12406	H	-4.46429	3.79868	-3.46861
H	-0.71873	-3.01993	2.42284	H	-4.24911	2.03553	-5.23352
H	-1.69015	-4.47752	2.76162	H	-2.47470	0.28006	-5.02406
H	-5.28240	-5.28778	-0.35226	H	-0.92676	0.29534	-3.06831
H	-5.47203	-3.66007	-1.03907	C	-1.10707	3.93628	1.35726
H	-5.06230	-5.02329	-2.10472	C	-1.87179	4.50736	2.38830
H	4.96311	-0.94937	-2.60273	C	-3.14819	4.00583	2.68403
H	4.46093	-2.56670	-2.06078	C	-3.65957	2.92588	1.94451
H	3.22519	-1.30725	-2.30206	C	-2.89651	2.35001	0.91830
H	7.74902	1.07598	0.82913	H	-0.11433	4.33789	1.13355
H	6.50429	2.26142	1.27357	H	-1.46489	5.34853	2.95946
H	7.17461	1.17893	2.51751	H	-3.74245	4.45160	3.48848
H	2.51530	-2.67762	2.73199	H	-4.65336	2.52502	2.17005
H	4.00202	-2.47854	3.69436	H	-3.30234	1.50533	0.35309
H	2.75037	-1.21635	3.71058	C	-0.74184	-3.30443	-2.34994
6ortho				C	-1.97773	-3.53091	-2.98157
SCF (BP86) Energy =				C	-3.10895	-3.97789	-2.27485
Enthalpy 0K =				C	-2.96387	-4.24410	-0.90343
Enthalpy 298K =				C	-1.75165	-4.03563	-0.21512
Free Energy 298K =				C	0.46523	-2.93094	-3.18206
SCRf (PCM, THF) Energy =				H	-2.04722	-3.37594	-4.06513
Ru	0.36221	-0.15636	-0.37575	C	-4.43793	-4.17121	-2.97248
C	1.20697	-2.03453	-0.08539	H	-3.81924	-4.63391	-0.33862
N	2.47977	-2.36324	0.35829	C	-1.65970	-4.42484	1.24374
C	2.64699	-3.74910	0.44841	C	3.89468	-0.81346	1.70829
C	1.48028	-4.32211	0.03970	C	5.04129	0.00810	1.76300
				C	5.90440	0.17359	0.67066

C	5.61388	-0.53111	-0.51407
C	4.48726	-1.35972	-0.62893
C	3.03825	-0.95869	2.94264
H	5.26402	0.52237	2.70605
C	7.12388	1.06670	0.75810
H	6.28681	-0.43973	-1.37524
C	4.24065	-2.12117	-1.91309
H	2.39706	-0.07051	3.07456
H	2.36909	-1.82778	2.89906
H	3.67486	-1.04144	3.84009
H	4.14684	-3.20697	-1.73652
H	3.31437	-1.78757	-2.40771
H	5.07092	-1.96164	-2.61874
H	8.04427	0.52065	0.48546
H	7.04271	1.92329	0.06508
H	7.25760	1.46931	1.77503
H	-2.62846	-4.26014	1.74290
H	-1.42495	-5.50201	1.33892
H	-0.89047	-3.86340	1.79185
H	-5.04508	-4.94799	-2.47932
H	-5.02964	-3.23745	-2.96097
H	-4.30290	-4.45817	-4.02865
H	1.35826	-3.49919	-2.87159
H	0.27605	-3.14348	-4.24642
H	0.72054	-1.86310	-3.08916

TS (6-3)_{ortho}

SCF (BP86) Energy =	-2563.731177		
Enthalpy 0K =	-2562.992973		
Enthalpy 298K =	-2562.935224		
Free Energy 298K =	-2563.088320		
SCRF (PCM,THF) Energy =	-2563.74438759		
Imaginary Frequency =	-101.1054	cm-1	
Ru	-0.11040	-0.41433	0.21454
C	0.28656	-2.48184	-0.08096
N	-0.72463	-3.40557	-0.33632
C	-0.22364	-4.69531	-0.50930
C	1.12790	-4.61658	-0.35228
N	1.42365	-3.27702	-0.09277
C	-2.15680	-3.17827	-0.37779
C	2.78972	-2.87480	0.16176
H	1.90690	-5.37289	-0.39468
H	-0.87753	-5.53579	-0.72500
C	-0.34148	-0.64053	1.97912
O	-0.36750	-0.77133	3.16198
P	-1.20946	1.70304	0.31426
C	-0.20033	3.25974	0.50432
C	-2.32929	2.01829	-1.14739
C	-2.43711	1.86091	1.72352
H	0.98434	-0.43133	-1.89582
H	-1.59457	-0.92170	0.10322
C	1.67278	0.59886	-0.82026
C	2.76790	0.43007	0.07612
C	3.78683	1.37991	0.19147
C	1.73480	1.76283	-1.60674
C	3.81797	2.51266	-0.63369
C	2.77846	2.69737	-1.55599
H	2.85017	-0.45459	0.71028
F	0.52015	-0.92295	-2.66860
F	4.80324	1.20956	1.08249
F	0.73720	2.04501	-2.49851
F	4.82827	3.40468	-0.55821
F	2.79167	3.77902	-2.36618
C	-3.37158	2.96797	-1.07278
C	-4.21331	3.18351	-2.17463
C	-4.02952	2.44512	-3.35576
C	-3.00269	1.49123	-3.42986
C	-2.15371	1.27418	-2.33196

H	-3.53186	3.53221	-0.14807
H	-5.01662	3.92501	-2.10714
H	-4.68876	2.61157	-4.21453
H	-2.85460	0.91148	-4.34694
H	-1.34989	0.53519	-2.40711
C	-2.50312	3.00067	2.54993
C	-3.46364	3.08173	3.57329
C	-4.37199	2.03252	3.77563
C	-4.31558	0.89654	2.95050
C	-3.35320	0.80749	1.93470
H	-1.80230	3.82702	2.39993
H	-3.49821	3.97124	4.21146
H	-5.11896	2.09682	4.57392
H	-5.01842	0.07053	3.10248
H	-3.30754	-0.08804	1.30573
C	-0.34076	4.38669	-0.32861
C	0.47245	5.51531	-0.13080
C	1.42202	5.53208	0.90234
C	1.56667	4.41015	1.73652
C	0.76748	3.27576	1.53321
H	-1.07632	4.38064	-1.13815
H	0.36322	6.38217	-0.79098
H	2.05555	6.41250	1.05222
H	2.31230	4.41206	2.53845
H	0.89907	2.39409	2.17012
C	3.24315	-2.82057	1.50071
C	4.58053	-2.44290	1.72103
C	5.45533	-2.14317	0.66069
C	4.97768	-2.27905	-0.65548
C	3.65095	-2.65155	-0.93753
C	2.33846	-3.15355	2.66653
H	4.94463	-2.37873	2.75333
C	6.86126	-1.65484	0.92935
H	5.65444	-2.08053	-1.49499
C	3.18154	-2.81180	-2.36575
C	-2.77987	-2.93937	-1.62539
C	-4.17678	-2.77576	-1.63566
C	-4.95152	-2.86923	-0.46489
C	-4.29607	-3.16825	0.74347
C	-2.90086	-3.33895	0.81509
C	-1.98678	-2.89434	-2.91018
H	-4.67233	-2.57915	-2.59388
C	-6.44928	-2.65361	-0.50690
H	-4.88590	-3.28722	1.66049
C	-2.23891	-3.68830	2.12845
H	-2.63703	-2.61761	-3.75501
H	-1.15233	-2.17676	-2.85326
H	-1.54547	-3.88194	-3.13961
H	-1.53079	-4.52764	2.01866
H	-1.66840	-2.83650	2.53546
H	-2.99423	-3.97476	2.87730
H	-6.95418	-3.14996	0.33812
H	-6.69600	-1.57745	-0.45218
H	-6.88738	-3.03859	-1.44297
H	3.98694	-2.54110	-3.06643
H	2.89050	-3.85667	-2.57854
H	2.30178	-2.18365	-2.58543
H	7.55224	-1.93197	0.11626
H	6.86427	-0.55313	1.00870
H	7.25945	-2.05677	1.87567
H	1.76600	-4.07953	2.48578
H	2.93091	-3.29204	3.58473
H	1.60320	-2.35461	2.86078

TS (2-3)_{ortho}

SCF (BP86) Energy =	-2563.682189
Enthalpy 0K =	-2562.946631
Enthalpy 298K =	-2562.888549

Free Energy 298K = -2563.043968
SCRF (PCM,THF) Energy = -2563.69462400
Imaginary Frequency = -540.1680 cm-1
Ru 0.49443 0.30329 0.33810
C 1.83226 -1.24255 0.71755
N 1.58298 -2.40620 1.43857
C 2.70687 -3.23754 1.48138
C 3.69771 -2.59885 0.79715
N 3.16459 -1.38697 0.34458
C 0.39915 -2.69851 2.22246
C 4.02363 -0.35677 -0.21161
H 4.72588 -2.88167 0.58786
H 2.68822 -4.19534 1.99383
C 1.55234 1.62699 1.08872
O 2.19863 2.51220 1.53473
P -1.30252 1.84806 0.16542
C -1.43377 2.78887 -1.44918
C -3.02736 1.17727 0.44577
C -1.27903 3.23460 1.42537
H -0.51576 -0.87621 -0.64372
H -0.09233 0.01109 1.75094
C -0.50015 -1.04657 -2.10520
C -1.72077 -0.62610 -2.72019
C -2.57234 -1.55117 -3.31842
C -0.10475 -2.38929 -2.37973
C -2.23118 -2.90703 -3.44829
C -0.98267 -3.31300 -2.94844
H -2.02223 0.42135 -2.66905
F 0.58214 -0.06879 -2.19966
F -3.75637 -1.13821 -3.83252
F 1.08699 -2.84484 -1.89291
F -3.06699 -3.80044 -4.02696
F -0.60848 -4.60868 -3.04632
C 4.24500 -0.27547 -1.60516
C 5.11792 0.72752 -2.07105
C 5.77496 1.61651 -1.20413
C 5.57426 1.46114 0.17956
C 4.71708 0.47775 0.70096
C 3.60766 -1.22986 -2.58644
H 5.29432 0.80204 -3.15099
C 6.67392 2.71002 -1.74013
H 6.10395 2.11885 0.87891
C 4.58568 0.29938 2.19708
H 3.53612 0.35558 2.52495
H 4.97577 -0.68290 2.51996
H 5.14878 1.08072 2.73031
H 4.12702 -1.18180 -3.55693
H 3.63895 -2.27061 -2.22706
H 2.54838 -0.97987 -2.74843
H 7.04761 2.46931 -2.74890
H 6.12998 3.66989 -1.81084
H 7.54320 2.87901 -1.08249
C -0.52480 -3.66961 1.77675
C -1.64822 -3.93070 2.58750
C -1.85420 -3.28414 3.81607
C -0.87609 -2.37078 4.25429
C 0.25998 -2.06813 3.48607
C -0.31972 -4.47134 0.51184
H -2.37694 -4.67475 2.24305
C -3.08967 -3.55554 4.64734
H -0.99289 -1.88516 5.23084
C 1.30813 -1.11927 4.02177
H 0.17099 -5.43654 0.73950
H -1.28518 -4.71045 0.03761
H 0.30840 -3.94980 -0.22042
H 1.31368 -0.17411 3.45175
H 1.11454 -0.88544 5.08070
H 2.32148 -1.55029 3.94478

H -3.54358 -4.52743 4.39345
H -2.85987 -3.55532 5.72630
H -3.85778 -2.77860 4.47917
C -3.25117 -0.21040 0.35222
C -4.53744 -0.73692 0.55491
C -5.60960 0.11601 0.85921
C -5.39192 1.49985 0.96890
C -4.10764 2.02884 0.76757
H -2.40463 -0.87186 0.13940
H -4.69799 -1.81734 0.47826
H -6.61188 -0.29574 1.01897
H -6.22171 2.16968 1.21888
H -3.94108 3.10574 0.87674
C -1.44305 4.59008 1.07908
C -1.43238 5.58266 2.07491
C -1.26589 5.23080 3.42246
C -1.10452 3.87969 3.77429
C -1.10568 2.88849 2.78289
H -1.57555 4.87493 0.03089
H -1.55524 6.63358 1.79159
H -1.25702 6.00546 4.19648
H -0.96815 3.59714 4.82367
H -0.96181 1.83778 3.05694
C -2.64595 3.05447 -2.11937
C -2.64249 3.74517 -3.34372
C -1.43339 4.18419 -3.90525
C -0.22160 3.92371 -3.24320
C -0.22022 3.22237 -2.02856
H -3.59426 2.71532 -1.69091
H -3.58986 3.93729 -3.85862
H -1.43383 4.72048 -4.86000
H 0.72672 4.25539 -3.67900
H 0.72763 2.99737 -1.52662

TS (2-3)_C6F6

SCF (BP86) Energy = -2662.90347870
Enthalpy 0K = -2662.176524
Enthalpy 298K = -2662.118176
Free Energy 298K = -2662.276246
SCRF (PCM,THF) Energy = -2662.91507517
Imaginary Frequency = -355.7047 cm-1
Ru -0.67697 0.06829 0.51416
C -2.42107 0.84623 -0.31990
N -2.80037 2.16755 -0.51320
C -4.08369 2.26018 -1.06262
C -4.54249 0.98544 -1.21887
N -3.53048 0.13736 -0.76299
C -2.05345 3.35150 -0.13959
C -3.70414 -1.29629 -0.64892
H -5.48409 0.60046 -1.60071
H -4.54243 3.22099 -1.27897
C -1.45448 -0.30515 2.15597
O -1.89927 -0.55451 3.22452
P 1.41887 -0.65781 1.35068
C 1.78428 -2.42559 0.87672
C 2.95412 0.30584 0.90331
C 1.62123 -0.67587 3.21479
H 0.26646 0.35278 -1.05038
H -0.33214 1.50360 0.99953
C 0.63630 0.22049 -2.46624
C 0.95739 -1.14857 -2.73062
C 2.24047 -1.56529 -3.08088
C 1.67358 1.14596 -2.79877
C 3.25626 -0.62211 -3.32149
C 2.96279 0.73900 -3.14805
F 0.01260 -2.08058 -2.42909
F -0.66536 0.62585 -2.87650
F 2.50722 -2.88164 -3.23247

F	1.43192	2.47057	-2.60221
F	4.49198	-1.02291	-3.69801
F	3.92273	1.66609	-3.35904
C	2.82125	1.49795	0.16694
C	3.95165	2.27882	-0.13035
C	5.22041	1.87534	0.31049
C	5.35906	0.69280	1.05877
C	4.23251	-0.08587	1.35994
H	1.82687	1.81428	-0.16303
H	3.83391	3.19465	-0.71738
H	6.10222	2.48100	0.07600
H	6.34649	0.37963	1.41445
H	4.34535	-0.99281	1.96336
C	1.24974	0.48905	3.91938
C	1.42856	0.56722	5.30790
C	1.97197	-0.52059	6.01189
C	2.33973	-1.68341	5.31832
C	2.17006	-1.76145	3.92524
H	0.81461	1.33398	3.37437
H	1.13438	1.47687	5.84224
H	2.10468	-0.46222	7.09737
H	2.76256	-2.53654	5.85990
C	2.46083	-2.67331	3.39447
C	2.86629	-2.81166	0.06109
C	3.02236	-4.15478	-0.32173
C	2.10683	-5.12556	0.11077
C	1.02130	-4.74851	0.91986
C	0.85300	-3.40695	1.29144
H	3.58726	-2.06397	-0.28213
H	3.86215	-4.43724	-0.96432
H	2.23326	-6.17175	-0.18692
H	0.29906	-5.49907	1.25822
H	-0.00160	-3.11815	1.91375
C	-4.22920	-1.82075	0.55626
C	-4.37632	-3.21759	0.65641
C	-4.05593	-4.07923	-0.40635
C	-3.61171	-3.50868	-1.61405
C	-3.43785	-2.12207	-1.76871
C	-4.72026	-0.93292	1.67905
H	-4.76776	-3.63718	1.59112
C	-4.18687	-5.58037	-0.26153
H	-3.39881	-4.15969	-2.47037
C	-3.05438	-1.54408	-3.11116
C	-1.42562	4.11822	-1.14882
C	-0.72904	5.27551	-0.75327
C	-0.66267	5.68990	0.58858
C	-1.35545	4.93294	1.55060
C	-2.06840	3.76834	1.21309
C	-1.52108	3.74867	-2.61137
H	-0.22922	5.87235	-1.52561
C	0.13051	6.91608	0.98716
H	-1.35711	5.26328	2.59652
C	-2.84955	3.02198	2.26995
H	-2.55867	3.83817	-2.98158
H	-0.89236	4.41811	-3.21853
H	-1.19768	2.71342	-2.79083
H	-2.36774	2.06427	2.52555
H	-2.92714	3.62249	3.19023
H	-3.87262	2.78777	1.92734
H	1.16831	6.64616	1.25636
H	0.18703	7.64743	0.16402
H	-0.31242	7.41811	1.86348
H	-2.78151	-2.34751	-3.81265
H	-3.90155	-0.98777	-3.55347
H	-2.20926	-0.84618	-3.03831
H	-4.54974	-6.04657	-1.19304
H	-3.21007	-6.04228	-0.02830
H	-4.88087	-5.85036	0.55118

H	-4.20191	0.03527	1.70911
H	-5.80081	-0.72915	1.55757
H	-4.58178	-1.42033	2.65625

TS (5-6)_C6F6

SCF (BP86) Energy =	-2662.89867181		
Enthalpy 0K =	-2662.169169		
Enthalpy 298K =	-2662.110860		
Free Energy 298K =	-2662.267593		
SCRF (PCM,THF) Energy =	-2662.91896543		
Imaginary Frequency =	-403.8224 cm-1		
Ru	0.31170	0.17495	-0.07350
C	1.74104	1.68075	-0.30510
N	1.44315	3.02249	-0.46350
C	2.59148	3.77749	-0.71710
C	3.63786	2.90516	-0.73311
N	3.11057	1.63158	-0.48703
C	0.12313	3.62567	-0.46377
C	3.95943	0.45990	-0.55560
H	4.70158	3.05422	-0.89579
H	2.54242	4.85432	-0.85182
C	1.41580	-1.23940	-0.15378
O	2.06783	-2.22614	-0.15291
P	-1.46845	-1.32632	-0.73192
C	-1.00588	-2.36296	-2.23184
C	-2.14059	-2.63100	0.41985
C	-2.98803	-0.44084	-1.35675
H	-0.96683	1.79772	1.56011
H	0.32216	0.32726	-1.66961
C	-0.71269	0.83579	2.03502
C	0.64618	0.46214	2.28460
C	0.91707	-0.69805	3.08611
C	-1.74238	-0.02521	2.51041
C	-0.10992	-1.48852	3.56166
C	-1.46108	-1.12437	3.29829
F	1.59177	1.45867	2.42587
F	-1.15404	2.39963	3.30058
F	2.20388	-1.00992	3.36556
F	-3.03149	0.28436	2.24390
F	0.13830	-2.62657	4.24650
F	-2.44502	-1.90654	3.78170
C	-3.51893	-2.81920	0.64109
C	-3.96305	-3.84401	1.49342
C	-3.03922	-4.68534	2.13069
C	-1.66259	-4.49535	1.92351
C	-1.21290	-3.47153	1.07679
H	-4.24711	-2.16929	0.14742
H	-5.03686	-3.97960	1.65987
H	-3.38881	-5.48057	2.79718
H	-0.93414	-5.13703	2.42902
H	-0.13814	-3.33010	0.92130
C	-3.81305	-1.01666	-2.34814
C	-4.95954	-0.34164	-2.79391
C	-5.29209	0.91441	-2.25916
C	-4.47322	1.49398	-1.27807
C	-3.32447	0.82229	-0.82982
H	-3.55675	-1.99218	-2.77299
H	-5.59279	-0.79883	-3.56161
H	-6.18711	1.43980	-2.60879
H	-4.72208	2.47185	-0.85488
H	-2.70236	1.28194	-0.05766
C	-1.19941	-3.75861	-2.27263
C	-0.86579	-4.49125	-3.42536
C	-0.34956	-3.84014	-4.55463
C	-0.16612	-2.44735	-4.52725
C	-0.48654	-1.71659	-3.37448
H	-1.60868	-4.28128	-1.40411
H	-1.01493	-5.57613	-3.43480

H	-0.09145	-4.41243	-5.45183	C	0.60978	-1.05551	-2.92051
H	0.23218	-1.92679	-5.40467	C	1.69273	-1.76479	-3.42318
H	-0.33052	-0.63308	-3.35767	C	1.91404	0.94469	-2.78252
C	4.07461	-0.20946	-1.79733	C	2.90836	-1.09593	-3.62936
C	4.94542	-1.30951	-1.87242	C	3.02380	0.25802	-3.28245
C	5.70008	-1.73782	-0.76551	F	-0.56042	-1.71176	-2.65272
C	5.59379	-1.01147	0.43364	F	-0.48646	1.10061	-2.79438
C	4.73899	0.09830	0.56737	H	1.59219	-2.82470	-3.66421
C	3.29696	0.24024	-3.01344	F	2.06510	2.24597	-2.40819
H	5.03672	-1.84322	-2.82599	F	3.98088	-1.74915	-4.14492
C	6.59561	-2.95396	-0.86036	F	4.19257	0.91752	-3.45388
H	6.19877	-1.31060	1.29788	C	2.13688	-3.56312	-0.43283
C	4.68580	0.86786	1.86743	C	1.95887	-4.83860	-0.99631
C	-0.32634	4.31764	0.68835	C	0.76486	-5.54594	-0.78850
C	-1.59961	4.92279	0.61642	C	-0.26069	-4.96971	-0.01964
C	-2.38262	4.89952	-0.54798	C	-0.08998	-3.69399	0.53731
C	-1.86715	4.25279	-1.68884	H	3.06970	-3.01967	-0.60759
C	-0.61165	3.62332	-1.67902	H	2.76072	-5.27822	-1.59935
C	0.45237	4.39969	1.97380	H	0.63088	-6.54045	-1.22704
H	-1.97660	5.43189	1.51091	H	-1.19839	-5.51147	0.14310
C	-3.72445	5.60084	-0.59179	H	-0.89734	-3.24611	1.12811
H	-2.44846	4.25169	-2.61844	C	4.07879	-1.42669	1.19733
C	-0.05353	3.01714	-2.94760	C	5.37365	-0.94032	0.96642
H	4.80152	1.95354	1.70677	C	5.55910	0.29371	0.31808
H	3.72321	0.72386	2.38099	C	4.44599	1.04402	-0.08791
H	5.49019	0.53526	2.54206	C	3.14723	0.55878	0.14276
H	7.44831	-2.88533	-0.16487	H	3.94197	-2.37706	1.72425
H	6.03697	-3.87276	-0.60397	H	6.23969	-1.52281	1.29861
H	6.99240	-3.08746	-1.88051	H	6.57158	0.66952	0.13615
H	3.61574	-0.32034	-3.90613	H	4.57832	2.00397	-0.59597
H	2.21359	0.08001	-2.87263	H	2.27607	1.15112	-0.15205
H	3.43958	1.31682	-3.21384	C	1.53835	-2.95221	3.44778
H	0.37280	5.41498	2.39832	C	1.68963	-3.15278	4.83102
H	-0.01414	3.67817	2.69474	C	1.68333	-2.05914	5.70951
H	1.51617	4.15339	1.84550	C	1.52103	-0.75904	5.20135
H	0.94305	3.42888	-3.18711	C	1.36123	-0.55645	3.82338
H	0.06580	1.92349	-2.85229	H	1.54648	-3.81256	2.77152
H	-0.72161	3.22006	-3.79937	H	1.81418	-4.16954	5.21911
H	-4.36077	5.20991	-1.40292	H	1.80092	-2.21786	6.78666
H	-4.26894	5.48879	0.36061	H	1.50991	0.09994	5.88072
H	-3.60068	6.68546	-0.76775	H	1.22223	0.45699	3.43097
TS (2-3)_C6F5H_2				C	-4.59144	-0.59090	0.51455
SCF (BP86) Energy =				C	-5.15936	-1.87782	0.46994
Enthalpy 0K =				C	-5.11560	-2.67193	-0.68947
Enthalpy 298K =				C	-4.51500	-2.13312	-1.84219
Free Energy 298K =				C	-3.92519	-0.85591	-1.85395
SCRF (PCM,THF) Energy =				C	-4.78146	0.27529	1.74062
Imaginary Frequency =				H	-5.66203	-2.26001	1.36666
Ru	-0.60241	0.12039	0.47146	C	-5.70082	-4.06811	-0.69928
C	-2.04865	1.48275	-0.15371	H	-4.51062	-2.71791	-2.76981
N	-2.01558	2.87026	-0.16615	C	-3.37906	-0.27550	-3.13742
C	-3.22266	3.41010	-0.62269	C	-0.14059	4.40104	-0.65286
C	-4.04838	2.36073	-0.89977	C	0.88005	5.24050	-0.16828
N	-3.33011	1.19864	-0.60836	C	1.10679	5.43019	1.20617
C	-0.93770	3.72037	0.29677	C	0.25019	4.78249	2.11468
C	-3.92985	-0.11930	-0.64495	C	-0.78665	3.93323	1.68809
H	-5.06987	2.32560	-1.26851	C	-0.38499	4.27724	-2.13938
H	-3.37419	4.48332	-0.69734	H	1.51197	5.76509	-0.89491
C	-1.45498	-0.26564	2.07026	C	2.24037	6.30608	1.69546
O	-1.95572	-0.53061	3.10975	H	0.37904	4.95201	3.19067
P	1.21326	-1.27519	1.10311	C	-1.72136	3.30738	2.69770
C	1.37119	-1.65180	2.93330	H	0.40862	4.79121	-2.70323
C	1.11774	-2.98246	0.34775	H	-0.41181	3.22584	-2.46001
C	2.95356	-0.68516	0.77180	H	-1.34904	4.73523	-2.42709
H	0.38890	0.36688	-1.09479	H	-2.77803	3.43261	2.40323
H	0.14376	1.30293	1.14971	H	-1.54016	2.22451	2.79576
C	0.66941	0.30662	-2.47844	H	-1.58630	3.76918	3.68870
				H	2.48882	7.09332	0.96461

H	1.99235	6.79229	2.65375
H	3.15779	5.71137	1.85981
H	-3.39122	-1.03155	-3.93771
H	-3.99635	0.57798	-3.47374
H	-2.35026	0.09323	-3.02398
H	-6.09509	-4.33469	-1.69399
H	-4.93409	-4.82156	-0.44099
H	-6.51806	-4.17031	0.03370
H	-3.94362	0.96813	1.90071
H	-5.70041	0.88321	1.64129
H	-4.88702	-0.34277	2.64527

TS (5-6) _C6F5H_2

SCF (BP86) Energy = -2563.69641458
Enthalpy 0K = -2562.960802
Enthalpy 298K = -2562.904361
Free Energy 298K = -2563.054507
SCRF (PCM,THF) Energy = -2563.70021017
Imaginary Frequency = -564.8691 cm-1

Ru	0.25647	0.12670	0.10761
C	1.53720	1.73616	-0.31555
N	1.21091	3.06096	-0.59446
C	2.33331	3.80418	-0.97507
C	3.39569	2.95528	-0.95048
N	2.90666	1.70768	-0.55137
C	-0.08076	3.71765	-0.55529
C	3.79744	0.56604	-0.56934
H	4.44717	3.10442	-1.17926
H	2.25537	4.85758	-1.22857
C	1.52069	-1.25458	-0.02629
O	2.19506	-2.22222	-0.00648
P	-1.37461	-1.52232	-0.52091
C	-0.77820	-2.67117	-1.88857
C	-2.01337	-2.75887	0.73148
C	-2.94950	-0.88022	-1.31286
H	-1.02666	1.21501	0.48413
H	0.04296	0.33015	-1.49308
C	-0.82835	0.98372	1.93249
C	0.52346	0.52291	2.27765
C	0.68160	-0.60707	3.16576
C	-1.92144	0.18593	2.48906
C	-0.40430	-1.27154	3.67689
C	-1.73242	-0.86468	3.34444
F	1.43455	1.55059	2.56750
F	-1.04338	2.35809	2.15953
F	1.94732	-0.98814	3.46967
F	-3.17551	0.60356	2.16590
F	-0.23521	-2.37213	4.45542
H	-2.58168	-1.43900	3.71972
C	-3.38002	-2.93264	1.02782
C	-3.78180	-3.85946	2.00559
C	-2.82625	-4.62455	2.69235
C	-1.46127	-4.45173	2.40712
C	-1.05576	-3.51872	1.44125
H	-4.13499	-2.34484	0.49821
H	-4.84768	-3.98287	2.22630
H	-3.14193	-5.34737	3.45204
H	-0.70693	-5.03180	2.94765
H	0.01138	-3.37872	1.23795
C	-3.77662	-1.75012	-2.05903
C	-4.95995	-1.27800	-2.64614
C	-5.33126	0.06948	-2.50039
C	-4.51008	0.94081	-1.76946
C	-3.32383	0.47009	-1.18183
H	-3.49024	-2.79892	-2.18829
H	-5.58977	-1.96389	-3.22279
H	-6.25376	0.43800	-2.96174
H	-4.78351	1.99499	-1.65636

H	-2.67566	1.16182	-0.63585
C	-0.96024	-4.06841	-1.84158
C	-0.54257	-4.87864	-2.91179
C	0.04990	-4.30493	-4.04589
C	0.22602	-2.91245	-4.10452
C	-0.18023	-2.10361	-3.03367
H	-1.42481	-4.53195	-0.96703
H	-0.68501	-5.96310	-2.85344
H	0.37389	-4.93760	-4.87903
H	0.68656	-2.45252	-4.98550
H	-0.02634	-1.02072	-3.07480
C	3.95046	-0.13006	-1.79229
C	4.87547	-1.18525	-1.83882
C	5.64703	-1.54588	-0.71888
C	5.49665	-0.79817	0.46168
C	4.58568	0.26994	0.56507
C	3.14265	0.24833	-3.01257
H	4.99370	-1.74100	-2.77678
C	6.60279	-2.71759	-0.78087
H	6.11026	-1.04673	1.33599
C	4.47901	1.05804	1.84999
C	-0.35825	4.58799	0.52586
C	-1.57710	5.28745	0.50985
C	-2.50062	5.15710	-0.54337
C	-2.15984	4.32628	-1.62511
C	-0.94735	3.61078	-1.66763
C	0.62476	4.78475	1.65809
H	-1.80906	5.95349	1.34963
C	-3.82261	5.89423	-0.50992
H	-2.84218	4.24838	-2.48030
C	-0.58132	2.80406	-2.89029
H	4.43608	2.14426	1.66292
H	3.56473	0.79581	2.40497
H	5.34615	0.85345	2.49796
H	7.43092	-2.60445	-0.06185
H	6.08184	-3.66123	-0.53566
H	7.03501	-2.83642	-1.78858
H	3.37654	-0.41889	-3.85680
H	2.06155	0.18159	-2.80027
H	3.34554	1.28702	-3.33072
H	0.15938	5.35644	2.47627
H	0.96686	3.81982	2.06027
H	1.51876	5.34390	1.32661
H	0.42306	3.07173	-3.26308
H	-0.55794	1.72468	-2.65504
H	-1.30756	2.97300	-3.70088
H	-4.26135	5.98582	-1.51713
H	-4.55691	5.36409	0.12403
H	-3.70988	6.90890	-0.09185

TS (2-3) _C6F5H_3

SCF (BP86) Energy = -2563.68641616
Enthalpy 0K = -2562.951492
Enthalpy 298K = -2562.894256
Free Energy 298K = -2563.050147
SCRF (PCM,THF) Energy = -2563.69831953
Imaginary Frequency = -398.0167 cm-1

Ru	-0.40786	0.33656	0.51480
C	-1.38562	2.08864	-0.05078
N	-0.89928	3.38606	-0.13813
C	-1.90208	4.28900	-0.50762
C	-3.05120	3.56928	-0.65315
N	-2.72904	2.23966	-0.37097
C	0.43928	3.83785	0.18282
C	-3.72901	1.19463	-0.29005
H	-4.06017	3.86958	-0.92232
H	-1.69901	5.35019	-0.62183
C	-1.14085	0.30468	2.21957

O	-1.57551	0.23484	3.31877
P	0.87934	-1.57722	1.05166
C	1.22070	-1.87497	2.87172
C	0.03644	-3.15412	0.51948
C	2.62719	-1.70518	0.40809
H	0.39528	0.18480	-1.12991
H	0.76385	1.22055	1.02477
C	0.49546	0.01470	-2.61641
C	-0.09292	-1.24198	-2.96298
C	0.66238	-2.28512	-3.49300
C	1.85317	0.17899	-3.02926
C	2.01587	-2.12419	-3.82762
C	2.59412	-0.87776	-3.55895
F	-1.38507	-1.45235	-2.58779
F	-0.32831	1.14977	-2.82390
F	0.05451	-3.47638	-3.72368
F	2.46509	1.36336	-2.75354
H	2.59371	-2.93665	-4.26847
F	3.90079	-0.66269	-3.85038
C	0.52208	-3.98215	-0.51190
C	-0.22090	-5.09699	-0.93571
C	-1.45028	-5.40006	-0.33217
C	-1.94549	-4.57566	0.69284
C	-1.21466	-3.45369	1.10896
H	1.47808	-3.75382	-0.99201
H	0.16402	-5.72332	-1.74644
H	-2.02546	-6.27121	-0.66307
H	-2.90643	-4.80236	1.16693
H	-1.61152	-2.81026	1.90214
C	3.41856	-2.85261	0.63778
C	4.75298	-2.88741	0.20889
C	5.31436	-1.77459	-0.44244
C	4.53799	-0.62729	-0.66055
C	3.19856	-0.59154	-0.23557
H	2.99529	-3.71506	1.16343
H	5.35834	-3.78219	0.38974
H	6.35701	-1.80445	-0.77643
H	4.96255	0.23994	-1.17505
H	2.58995	0.30398	-0.39570
C	1.12195	-3.14105	3.48198
C	1.45169	-3.30175	4.83853
C	1.89107	-2.20442	5.59470
C	1.99680	-0.94056	4.99040
C	1.65947	-0.77533	3.63923
H	0.77927	-4.00388	2.90233
H	1.36441	-4.29013	5.30272
H	2.14694	-2.33191	6.65188
H	2.33429	-0.07778	5.57458
H	1.72983	0.21340	3.17271
C	-4.37171	0.96904	0.95068
C	-5.32905	-0.06109	1.01734
C	-5.67868	-0.82782	-0.10737
C	-5.07245	-0.51660	-1.33882
C	-4.10454	0.49582	-1.46320
C	-4.13305	1.85246	2.15587
H	-5.82261	-0.25611	1.97717
C	-6.68138	-1.95690	-0.00138
H	-5.36400	-1.07266	-2.23782
C	-3.55151	0.86396	-2.82026
C	1.31853	4.19036	-0.86742
C	2.60262	4.64982	-0.51947
C	3.01500	4.78369	0.81794
C	2.08646	4.48273	1.83073
C	0.78953	4.02108	1.54208
C	0.90017	4.12233	-2.31826
H	3.29704	4.91571	-1.32546
C	4.41789	5.23886	1.15898
H	2.37017	4.62462	2.88072

C	-0.19520	3.77071	2.66101
H	1.75451	4.34618	-2.97550
H	0.51241	3.12825	-2.58245
H	0.10491	4.85664	-2.54195
H	-1.17306	4.23857	2.45164
H	-0.37721	2.69292	2.80313
H	0.18390	4.18261	3.60980
H	4.83796	5.88371	0.36944
H	4.44294	5.79795	2.10923
H	5.09823	4.37464	1.27140
H	-3.88680	0.14268	-3.58141
H	-3.90603	1.86502	-3.12839
H	-2.45348	0.89049	-2.82901
H	-7.31125	-2.02490	-0.90431
H	-6.17008	-2.93056	0.11050
H	-7.34325	-1.83095	0.87110
H	-3.11766	2.27169	2.17715
H	-4.84317	2.70079	2.15345
H	-4.28699	1.29235	3.09085

TS(5-6)_C6F5H_3

SCF (BP86) Energy =	-2563.69762182	
Enthalpy 0K =	-2562.961862	
Enthalpy 298K =	-2562.905461	
Free Energy 298K =	-2563.055797	
SCRF (PCM,THF) Energy =	-2563.69954516	
Imaginary Frequency =	-602.2211	cm-1
Ru	-0.31523	0.06764 -0.11356
C	-1.92935	1.36612 0.24792
N	-1.91191	2.71662 0.59285
C	-3.18800	3.18812 0.91905
C	-4.04174	2.13761 0.79248
N	-3.27511	1.04088 0.38737
C	-0.79732	3.64086 0.66015
C	-3.90860	-0.25908 0.30972
H	-5.11275	2.05142 0.95283
H	-3.35127	4.22113 1.21265
C	-1.29103	-1.53909 -0.10848
O	-1.75611	-2.62071 -0.18699
P	1.55765	-1.29760 0.52034
C	1.16144	-2.51974 1.90260
C	2.34858	-2.44419 -0.73460
C	3.02930	-0.43285 1.30065
H	0.72842	1.41878 -0.27699
H	-0.27118	0.24338 1.50161
C	0.70515	1.25317 -1.79948
C	-0.43346	0.46590 -2.29056
C	-0.16637	-0.63778 -3.18395
C	2.02992	0.84500 -2.25693
C	1.09365	-0.98379 -3.59789
C	2.18987	-0.18549 -3.14825
F	-1.54737	1.22640 -2.67775
F	0.54037	2.63644 -1.94022
F	-1.24863	-1.33797 -3.60815
F	3.08112	1.61115 -1.86773
H	1.28167	-1.87473 -4.19813
F	3.43101	-0.48506 -3.60047
C	3.69871	-2.35649 -1.12686
C	4.22063	-3.24165 -2.08592
C	3.40436	-4.22780 -2.65869
C	2.05332	-4.31631 -2.28046
C	1.52448	-3.42455 -1.33562
H	4.34873	-1.59429 -0.68812
H	5.27046	-3.15375 -2.38467
H	3.81525	-4.92064 -3.40068
H	1.40430	-5.07797 -2.72589
H	0.46857	-3.49907 -1.05665
C	4.05603	-1.18706 1.91321

C	5.14816	-0.54597	2.51520	C	2.95967	3.38215	-0.77987
C	5.22695	0.85737	2.52158	C	3.91309	2.51097	-0.34375
C	4.20551	1.61265	1.92771	N	3.27524	1.28427	-0.12593
C	3.11094	0.97163	1.32280	C	0.56947	3.25852	-1.42570
H	3.99706	-2.28012	1.92828	C	4.04574	0.07609	0.10805
H	5.93593	-1.14426	2.98541	H	4.97850	2.63708	-0.17022
H	6.07888	1.35737	2.99468	H	3.01747	4.42868	-1.06685
H	4.25164	2.70658	1.93335	C	1.26396	-1.23725	-1.54871
H	2.30606	1.56697	0.88192	O	1.76909	-2.00445	-2.29523
C	1.65599	-3.84083	1.90874	P	-1.50983	-1.47200	-0.48958
C	1.39669	-4.69643	2.99304	C	-1.56303	-2.99696	0.59460
C	0.64987	-4.24367	4.09038	C	-3.17959	-0.65513	-0.26784
C	0.16081	-2.92724	4.09659	C	-1.75283	-2.21276	-2.19786
C	0.41137	-2.07491	3.01120	H	-0.30394	0.85428	1.04437
H	2.24030	-4.21210	1.06233	H	-0.21332	0.64952	-1.54664
H	1.78304	-5.72125	2.97446	C	-0.00392	0.63382	2.48165
H	0.44834	-4.91170	4.93450	C	-1.18455	0.19095	3.15195
H	-0.42377	-2.56125	4.94757	C	-1.79838	0.94754	4.15177
H	0.01490	-1.05474	3.01115	C	0.64488	1.76491	3.06409
C	-4.00557	-1.01804	1.50037	C	-1.17416	2.10969	4.63850
C	-4.69821	-2.23856	1.44923	C	0.04639	2.50980	4.09061
C	-5.29583	-2.70405	0.26380	F	-1.79492	-0.94298	2.72828
C	-5.21311	-1.89764	-0.88473	F	0.88603	-0.47211	2.09648
C	-4.53404	-0.66511	-0.89036	F	-2.96293	0.52188	4.68778
C	-3.37980	-0.53455	2.78850	H	1.59480	2.09085	2.63811
H	-4.76890	-2.84238	2.36192	F	-1.77195	2.81502	5.63316
C	-5.99597	-4.04513	0.22307	H	0.53686	3.40319	4.48695
H	-5.69644	-2.23143	-1.81085	C	4.36676	-0.32995	1.42302
C	-4.49612	0.18137	-2.14120	C	5.13760	-1.49839	1.57953
C	-0.66776	4.60624	-0.36680	C	5.60126	-2.24493	0.48353
C	0.36082	5.55648	-0.24974	C	5.31725	-1.76821	-0.80924
C	1.23697	5.57804	0.85092	C	4.55957	-0.60466	-1.02442
C	1.03702	4.63712	1.87609	C	3.93913	0.44931	2.64451
C	0.01399	3.67068	1.81777	H	5.38781	-1.82472	2.59629
C	-1.60685	4.63247	-1.55239	C	6.38632	-3.52323	0.68497
H	0.48020	6.29979	-1.04717	H	5.70392	-2.30969	-1.68072
C	2.36234	6.58787	0.92599	C	4.37032	-0.07222	-2.42738
H	1.67632	4.66754	2.76684	H	3.33146	0.23464	-2.61788
C	-0.22607	2.74440	2.98564	H	5.01130	0.81181	-2.60259
H	-4.77594	1.22879	-1.93375	H	4.63966	-0.83679	-3.17182
H	-3.48562	0.20533	-2.57821	H	4.60914	0.23326	3.49224
H	-5.19261	-0.21660	-2.89607	H	3.95607	1.53699	2.46363
H	-6.78130	-4.06974	-0.55045	H	2.91353	0.18010	2.94314
H	-5.27988	-4.85422	-0.01065	H	6.88251	-3.54340	1.66917
H	-6.45980	-4.29081	1.19303	H	5.72316	-4.40622	0.63310
H	-3.53305	-1.26798	3.59545	H	7.15796	-3.65205	-0.09247
H	-2.29518	-0.37608	2.65881	C	-0.25638	4.10683	-0.65568
H	-3.81006	0.42941	3.11530	C	-1.36670	4.69690	-1.28789
H	-1.24458	5.34029	-2.31441	C	-1.66210	4.47348	-2.64403
H	-1.68928	3.63750	-2.01520	C	-0.79073	3.65482	-3.38534
H	-2.62456	4.94865	-1.25964	C	0.33480	3.04309	-2.80512
H	-1.28069	2.77429	3.31189	C	0.03202	4.38762	0.79917
H	-0.00729	1.69772	2.70767	H	-2.01538	5.35536	-0.69761
H	0.40813	3.02365	3.84180	C	-2.88681	5.08863	-3.28652
H	2.70784	6.73352	1.96272	H	-0.98273	3.49285	-4.45301
H	3.23312	6.25619	0.33110	C	1.25774	2.18983	-3.64434
H	2.05379	7.56871	0.52638	H	1.05440	4.77762	0.94901
TS (2-3)_1,2,3,4-C6F4H2_1				H	-0.67570	5.13004	1.20057
SCF (BP86) Energy =				H	-0.05047	3.47323	1.41071
Enthalpy 0K =				H	1.17564	1.12750	-3.35485
Enthalpy 298K =				H	1.00586	2.27760	-4.71301
Free Energy 298K =				H	2.31439	2.48232	-3.51570
SCRF (PCM,THF) Energy =				H	-3.16971	6.03488	-2.79638
Imaginary Frequency =				H	-2.72364	5.29178	-4.35802
Ru 0.43354 -0.10169 -0.34281				H	-3.75548	4.40894	-3.21165
C	1.91262	1.35370	-0.41604	C	-3.25943	0.59248	0.38050
N	1.75382	2.67410	-0.82712	C	-4.50055	1.22556	0.55559
				C	-5.67462	0.62018	0.08130

C	-5.60285	-0.61655	-0.58129
C	-4.36263	-1.24852	-0.76169
H	-2.33765	1.07022	0.72765
H	-4.54735	2.19552	1.06190
H	-6.64262	1.11394	0.21852
H	-6.51321	-1.08829	-0.96670
H	-4.31234	-2.19867	-1.30383
C	-1.92537	-3.59307	-2.41812
C	-2.10573	-4.08791	-3.72213
C	-2.12350	-3.21052	-4.81587
C	-1.95573	-1.83120	-4.60282
C	-1.76700	-1.33623	-3.30491
H	-1.91628	-4.28684	-1.57218
H	-2.23273	-5.16469	-3.87812
H	-2.26413	-3.59763	-5.83067
H	-1.96591	-1.13867	-5.45152
H	-1.62095	-0.26245	-3.14479
C	-2.73934	-3.53104	1.15718
C	-2.68210	-4.68568	1.95464
C	-1.45307	-5.32043	2.19537
C	-0.27600	-4.79132	1.64141
C	-0.32928	-3.63261	0.85164
H	-3.70098	-3.03750	0.98751
H	-3.60259	-5.08611	2.39307
H	-1.41172	-6.21942	2.81955
H	0.68862	-5.27381	1.83173
H	0.59218	-3.20878	0.43724

TS (5-6)_1,2,3,4-C6F4H2_1

SCF (BP86) Energy =	-2464.46200617		
Enthalpy 0K =	-2463.715561		
Enthalpy 298K =	-2463.659762		
Free Energy 298K =	-2463.811003		
SCRf (PCM,THF) Energy =	-2464.47757416		
Imaginary Frequency =	-188.8041 cm-1		
Ru	-0.22100	0.33632	0.37651
C	-1.60186	1.91558	0.07849
N	-1.24604	3.21304	-0.25015
C	-2.36297	4.03847	-0.37786
C	-3.45514	3.26614	-0.11342
N	-2.98366	1.98310	0.16724
C	0.09585	3.73762	-0.41296
C	-3.89664	0.90759	0.50152
H	-4.51595	3.49920	-0.09239
H	-2.26851	5.08794	-0.64190
C	-0.42984	0.37258	2.17349
O	-0.56046	0.39296	3.35041
P	1.62118	-1.16668	0.68845
C	2.51485	-0.97722	2.32662
C	1.18328	-2.97765	0.65682
C	3.07915	-0.98826	-0.46536
H	-0.10597	0.55055	-1.59926
H	0.84604	1.47707	0.56221
C	-0.57515	-0.43449	-1.93423
C	-1.48559	-1.18772	-1.13692
C	-1.71602	-2.56265	-1.37940
C	0.20117	-1.15959	-2.87683
C	-1.01147	-3.20952	-2.38328
C	-0.05225	-2.50159	-3.14455
H	-2.19251	-0.66365	-0.47619
F	-1.54683	0.90848	-2.89212
H	-2.45885	-3.11366	-0.79823
F	1.15617	-0.51544	-3.59435
F	-1.21575	-4.52117	-2.67014
F	0.65560	-3.14747	-4.09616
C	1.61700	-3.86318	-0.34943
C	1.17274	-5.19674	-0.35977
C	0.29626	-5.65880	0.63266

C	-0.14868	-4.77876	1.63438
C	0.28202	-3.44450	1.64089
H	2.29605	-3.51445	-1.13263
H	1.51083	-5.87112	-1.15299
H	-0.04734	-6.69837	0.62204
H	-0.83888	-5.12908	2.40927
H	-0.08289	-2.76080	2.41545
C	4.19794	-1.84522	-0.36017
C	5.31676	-1.65182	-1.18223
C	5.33779	-0.59333	-2.10740
C	4.23870	0.27220	-2.20253
C	3.11346	0.07746	-1.38399
H	4.19851	-2.65851	0.37284
H	6.17652	-2.32466	-1.09568
H	6.21327	-0.44285	-2.74784
H	4.24825	1.10135	-2.91705
H	2.26424	0.76288	-1.45371
C	2.93940	-2.07637	3.09947
C	3.66419	-1.87088	4.28562
C	3.97941	-0.57007	4.70619
C	3.56508	0.52923	3.93596
C	2.83439	0.32849	2.75585
H	2.69975	-3.09566	2.78202
H	3.98251	-2.73394	4.88017
H	4.54347	-0.41235	5.63146
H	3.80440	1.54820	4.25814
H	2.50409	1.18841	2.16312
C	-4.14828	0.61155	1.86041
C	-5.02985	-0.45026	2.14788
C	-5.67638	-1.17680	1.13528
C	-5.45902	-0.79228	-0.20236
C	-4.58864	0.25512	-0.55431
C	-3.58141	1.42862	3.00203
H	-5.22533	-0.69853	3.19836
C	-6.58999	-2.33736	1.46787
H	-5.99203	-1.31549	-1.00526
C	-4.44173	0.68277	-1.99545
C	0.61321	3.91431	-1.71807
C	1.91767	4.43908	-1.82561
C	2.67802	4.81021	-0.70321
C	2.09202	4.68010	0.57041
C	0.79936	4.15578	0.74268
C	-0.19711	3.60921	-2.95511
H	2.33947	4.57658	-2.82861
C	4.08767	5.34085	-0.85666
H	2.64980	5.00609	1.45682
C	0.18832	4.05887	2.12239
H	0.42765	3.72443	-3.85557
H	-0.64207	2.58979	-2.95160
H	-1.04143	4.31771	-3.05128
H	-0.83490	4.47256	2.14494
H	0.11870	3.01044	2.45939
H	0.79605	4.61268	2.85550
H	4.31448	6.11265	-0.10192
H	4.83174	4.53325	-0.72882
H	4.24843	5.77960	-1.85507
H	-4.99664	-0.00651	-2.65195
H	-4.86765	1.69268	-2.14578
H	-3.38388	0.72651	-2.33418
H	-7.46249	-2.37103	0.79390
H	-6.06126	-3.30231	1.36048
H	-6.95869	-2.27875	2.50503
H	-2.89299	2.21299	2.65773
H	-4.40269	1.91767	3.55635
H	-3.03223	0.79548	3.71649

TS (2-3)_1,2,3,4-C6F4H2_2

SCF (BP86) Energy =	-2464.45907398
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Enthalpy 0K = -2463.715598
Enthalpy 298K = -2463.659488
Free Energy 298K = -2463.811518
SCRF (PCM,THF) Energy = -2464.46578073
Lowest frequency = -566.7216 cm-1

Ru 0.39364 -0.09588 -0.27296
C 1.93709 1.29559 -0.30783
N 1.83754 2.64789 -0.62149
C 3.08007 3.28723 -0.55741
C 3.99597 2.33772 -0.21548
N 3.30023 1.13208 -0.07411
C 0.66720 3.32903 -1.13778
C 4.01285 -0.12806 0.04061
H 5.07003 2.39627 -0.06079
H 3.18599 4.34891 -0.76240
C 1.16505 -1.19395 -1.55344
O 1.62394 -1.93080 -2.35763
P -1.59163 -1.40400 -0.45242
C -1.67826 -2.96229 0.58150
C -3.23888 -0.54987 -0.20921
C -1.85940 -2.08374 -2.18265
H -0.33108 0.83650 1.12712
H -0.25324 0.73829 -1.41506
C -0.14928 0.56968 2.61220
C -1.38185 0.17524 3.21216
C -2.06143 0.99058 4.12214
C 0.44852 1.70995 3.23123
C -1.48889 2.16654 4.61769
C -0.21192 2.52290 4.14424
F -1.96331 -0.97139 2.78239
F 0.73549 -0.52301 2.29460
F -3.27659 0.57929 4.56180
F 1.68568 2.08441 2.77530
H -2.02736 2.77114 5.34942
H 0.29743 3.41924 4.50797
C 4.31834 -0.67292 1.30876
C 5.03737 -1.88375 1.34496
C 5.46791 -2.53918 0.17918
C 5.20062 -1.92884 -1.05954
C 4.49065 -0.72007 -1.15575
C 3.93379 0.00957 2.59947
H 5.27554 -2.31748 2.32378
C 6.19941 -3.86237 0.25161
H 5.55969 -2.40023 -1.98210
C 4.30158 -0.05672 -2.50177
H 3.25284 0.22599 -2.67786
H 4.90599 0.86569 -2.57921
H 4.61062 -0.73320 -3.31327
H 4.49244 -0.42770 3.44245
H 4.14245 1.09095 2.56857
H 2.85854 -0.10092 2.80219
H 6.69226 -4.00004 1.22808
H 5.50113 -4.70832 0.11362
H 6.96705 -3.94508 -0.53609
C -0.05458 4.22018 -0.31458
C -1.17332 4.87364 -0.87050
C -1.56490 4.68555 -2.20474
C -0.78047 3.83741 -3.01054
C 0.34071 3.15729 -2.50825
C 0.36221 4.53825 1.10317
H -1.74720 5.55777 -0.23330
C -2.79327 5.36950 -2.76561
H -1.04116 3.70832 -4.06816
C 1.17910 2.29455 -3.42379
H 1.01704 3.76777 1.52896
H 0.90593 5.50120 1.13931
H -0.51968 4.64186 1.75614
H 1.06183 1.22553 -3.17567

H 0.88204 2.44085 -4.47440
H 2.25298 2.53394 -3.33409
H -3.07177 6.25442 -2.17031
H -2.63595 5.69302 -3.80854
H -3.66161 4.68545 -2.76581
C -3.27809 0.70669 0.42507
C -4.50042 1.37390 0.60684
C -5.69526 0.79381 0.15367
C -5.66359 -0.45163 -0.49597
C -4.44242 -1.11719 -0.68406
H -2.33971 1.16339 0.75626
H -4.51558 2.35050 1.10211
H -6.64858 1.31396 0.29637
H -6.59036 -0.90321 -0.86614
H -4.42272 -2.07234 -1.21941
C -2.02916 -3.45531 -2.45233
C -2.22407 -3.90154 -3.77174
C -2.25883 -2.98391 -4.83145
C -2.09409 -1.61274 -4.56884
C -1.89158 -1.16620 -3.25562
H -2.00662 -4.18031 -1.63326
H -2.34921 -4.97222 -3.96649
H -2.41071 -3.33324 -5.85826
H -2.11809 -0.88880 -5.39063
H -1.75107 -0.09797 -3.05728
C -2.86061 -3.48041 1.14622
C -2.82491 -4.66201 1.90433
C -1.61178 -5.34031 2.10354
C -0.42841 -4.82765 1.54766
C -0.46007 -3.64221 0.79724
H -3.80953 -2.95313 1.01066
H -3.74984 -5.04953 2.34501
H -1.58746 -6.26052 2.69691
H 0.52437 -5.34420 1.70543
H 0.46703 -3.23285 0.38041

TS(5-6)_1,2,3,4-C6F4H2_2

SCF (BP86) Energy = -2464.44839511
Enthalpy 0K = -2463.702970
Enthalpy 298K = -2463.646722
Free Energy 298K = -2463.798772
SCRF (PCM,THF) Energy = -2464.46891197
Imaginary Frequency = -387.9819 cm-1

Ru 0.34292 0.10136 0.07872
C 1.83772 1.51540 -0.22766
N 1.60209 2.85489 -0.49139
C 2.78746 3.54176 -0.76805
C 3.79630 2.62941 -0.69397
N 3.21054 1.39857 -0.37301
C 0.30798 3.50297 -0.60587
C 4.00631 0.18868 -0.36225
H 4.86852 2.72428 -0.84046
H 2.78754 4.60671 -0.98265
C 1.38258 -1.36160 0.11903
O 1.99223 -2.37245 0.20919
P -1.50967 -1.35356 -0.49295
C -1.07514 -2.46875 -1.94575
C -2.24327 -2.58304 0.70433
C -2.99014 -0.44422 -1.17815
H -0.82691 1.76329 1.50455
H 0.35922 0.12787 -1.51156
C -0.58660 0.92335 2.18331
C 0.74521 0.61564 2.58832
C 1.03100 -0.43767 3.49474
C -1.60185 0.04967 2.66728
C 0.00021 -1.23792 3.97338
C -1.32471 -0.96598 3.56885
F 1.69571 1.61002 2.50751

F	-1.13703	2.59368	3.17265
H	2.06113	-0.57646	3.83177
F	-2.88299	0.27256	2.28792
H	0.18418	-2.06372	4.66459
F	-2.34184	-1.71815	4.05315
C	-3.63029	-2.71588	0.90998
C	-4.12296	-3.68834	1.79568
C	-3.23874	-4.53646	2.47866
C	-1.85382	-4.40114	2.28640
C	-1.35498	-3.42374	1.41256
H	-4.32773	-2.06180	0.37907
H	-5.20319	-3.77941	1.95072
H	-3.62588	-5.29423	3.16783
H	-1.15645	-5.05136	2.82500
H	-0.27364	-3.31874	1.27569
C	-3.83500	-1.04203	-2.13963
C	-4.95215	-0.34859	-2.62947
C	-5.23573	0.94833	-2.16912
C	-4.39739	1.54971	-1.21808
C	-3.27790	0.85927	-0.72622
H	-3.61736	-2.05000	-2.50633
H	-5.60128	-0.82371	-3.37272
H	-6.10819	1.48793	-2.55270
H	-4.60879	2.55871	-0.85126
H	-2.64217	1.33577	0.02409
C	-1.22177	-3.86923	-1.90016
C	-0.89364	-4.65791	-3.01733
C	-0.43068	-4.05890	-4.19713
C	-0.29567	-2.66131	-4.25668
C	-0.61001	-1.87475	-3.13967
H	-1.59160	-4.35245	-0.99194
H	-1.00656	-5.74571	-2.95916
H	-0.17811	-4.67453	-5.06684
H	0.05807	-2.18054	-5.17505
H	-0.49610	-0.78712	-3.19461
C	4.08720	-0.57203	-1.55331
C	4.90758	-1.71288	-1.55039
C	5.64341	-2.09905	-0.41579
C	5.57201	-1.28786	0.73031
C	4.77200	-0.13159	0.78228
C	3.32500	-0.17848	-2.79785
H	4.97075	-2.31598	-2.46407
C	6.47890	-3.36078	-0.42529
H	6.16234	-1.55512	1.61509
C	4.77915	0.74799	2.01192
C	-0.16922	4.30813	0.45747
C	-1.40783	4.95873	0.26327
C	-2.12934	4.86903	-0.93592
C	-1.58565	4.10573	-1.98905
C	-0.36270	3.42988	-1.85689
C	0.54293	4.46679	1.77261
H	-1.80608	5.55958	1.08905
C	-3.43100	5.62178	-1.11783
H	-2.11712	4.04950	-2.94646
C	0.23579	2.70245	-3.04043
H	5.32064	1.69379	1.82469
H	3.76147	1.02180	2.32665
H	5.28621	0.24004	2.84761
H	7.32093	-3.29570	0.28339
H	5.87058	-4.23629	-0.13294
H	6.88784	-3.56892	-1.42807
H	3.64065	-0.79255	-3.65584
H	2.23858	-0.31557	-2.65567
H	3.48500	0.88323	-3.05518
H	0.46548	5.51099	2.12037
H	0.02341	3.80558	2.51697
H	1.60546	4.18952	1.71779
H	1.24917	3.07612	-3.27278

H	0.33140	1.62045	-2.84294
H	-0.39180	2.83838	-3.93530
H	-4.10484	5.10266	-1.81984
H	-3.96059	5.74951	-0.15954
H	-3.25172	6.63269	-1.52896

TS (2-3)_1,2,3,5-C6F4H2_1

SCF (BP86) Energy =	-2464.46093802		
Enthalpy 0K =	-2463.717798		
Enthalpy 298K =	-2463.661615		
Free Energy 298K =	-2463.814510		
SCRF (PCM,THF) Energy =	-2464.47307041		
Imaginary Frequency =	-599.3946 cm-1		
Ru	0.33901	-0.16236	-0.36085
C	1.95859	1.12144	-0.57503
N	1.91304	2.45633	-0.96604
C	3.19027	3.02407	-1.02711
C	4.07511	2.04604	-0.68293
N	3.32521	0.89591	-0.41138
C	0.75321	3.18126	-1.44793
C	3.97180	-0.39402	-0.25013
H	5.15919	2.04997	-0.60664
H	3.33934	4.06147	-1.31422
C	0.91033	-1.36338	-1.65304
O	1.24507	-2.16886	-2.45290
P	-1.74791	-1.30926	-0.30906
C	-1.85692	-2.82933	0.77743
C	-3.28735	-0.31781	0.07918
C	-2.24228	-2.00271	-1.98257
H	-0.15799	0.85117	1.07287
H	-0.33919	0.67832	-1.48445
C	0.27303	0.58230	2.50095
C	-0.88836	0.28718	3.27623
C	-1.31509	1.14464	4.29072
C	1.09700	1.64664	2.97790
C	-0.55929	2.25305	4.69962
C	0.64244	2.46308	4.01246
F	-1.65031	-0.78347	2.93807
F	0.98438	-0.60091	2.04511
F	-2.47689	0.85552	4.92410
H	2.03789	1.87317	2.47738
H	-0.89367	2.90553	5.50619
F	1.41914	3.52068	4.37720
C	4.37237	-0.84394	1.02823
C	5.01443	-2.09499	1.11220
C	5.27813	-2.88176	-0.02125
C	4.92629	-2.36496	-1.28167
C	4.29133	-1.11991	-1.42541
C	4.16376	-0.02913	2.28339
H	5.32478	-2.45546	2.10045
C	5.92612	-4.24365	0.10634
H	5.16159	-2.93996	-2.18512
C	4.03274	-0.55555	-2.80460
H	3.02162	-0.13296	-2.89741
H	4.74958	0.25341	-3.03864
H	4.14464	-1.33758	-3.57088
H	4.89709	-0.31654	3.05403
H	4.27292	1.05165	2.09462
H	3.15571	-0.19185	2.69656
H	6.50370	-4.33174	1.04113
H	5.16404	-5.04447	0.11396
H	6.60439	-4.45075	-0.73838
C	0.11428	4.11621	-0.60368
C	-0.97393	4.83931	-1.12687
C	-1.42488	4.66357	-2.44671
C	-0.73410	3.75293	-3.26677
C	0.36174	3.00703	-2.79722
C	0.57488	4.34857	0.81472

H	-1.47859	5.56560	-0.47834	H	0.89079	1.37130	0.60977
C	-2.62396	5.42581	-2.96865	C	-0.58835	-0.36488	-1.97303
H	-1.04699	3.62395	-4.31007	C	-1.53487	-1.11071	-1.21279
C	1.09239	2.05979	-3.72096	C	-1.78315	-2.45233	-1.55355
H	1.64090	4.63255	0.86304	C	0.15990	-1.05309	-2.95642
H	-0.01028	5.15193	1.28901	C	-1.12695	-3.10764	-2.59157
H	0.46270	3.43694	1.42513	C	-0.15236	-2.37045	-3.28979
H	0.91377	1.01119	-3.42521	H	-2.24566	-0.61354	-0.53696
H	0.75172	2.18880	-4.76044	F	-1.53830	1.12834	-2.86335
H	2.18361	2.22469	-3.69466	F	-2.72776	-3.12720	-0.84687
H	-2.74565	6.39253	-2.45263	F	1.13650	-0.40239	-3.64116
H	-2.54014	5.62181	-4.05061	H	-1.34874	-4.14077	-2.85963
H	-3.55570	4.85174	-2.81220	F	0.54000	-2.97017	-4.28568
C	-3.16594	0.92636	0.72756	C	1.99282	-3.84844	-0.68698
C	-4.30742	1.68905	1.02289	C	1.64493	-5.19494	-0.88917
C	-5.58171	1.21801	0.67057	C	0.57496	-5.76446	-0.18235
C	-5.71124	-0.01500	0.00974	C	-0.16055	-4.97940	0.72173
C	-4.57121	-0.77642	-0.29102	C	0.17504	-3.63176	0.91571
H	-2.16789	1.29842	0.98013	H	2.82788	-3.41560	-1.24513
H	-4.19758	2.65496	1.52717	H	2.21428	-5.79711	-1.60510
H	-6.47180	1.81320	0.90118	H	0.30844	-6.81480	-0.34063
H	-6.70132	-0.38267	-0.28078	H	-1.00602	-5.41112	1.26707
H	-4.67860	-1.72276	-0.83151	H	-0.41764	-3.01737	1.60256
C	-2.59424	-3.35194	-2.18076	C	4.35768	-1.56435	-0.22634
C	-2.96033	-3.81090	-3.45870	C	5.50597	-1.24747	-0.96582
C	-2.98622	-2.92742	-4.54738	C	5.46211	-0.22924	-1.93424
C	-2.63972	-1.57863	-4.35593	C	4.26796	0.47193	-2.15565
C	-2.26590	-1.12043	-3.08488	C	3.11456	0.15373	-1.41903
H	-2.58066	-4.04980	-1.33823	H	4.40556	-2.34178	0.54340
H	-3.22580	-4.86444	-3.59837	H	6.43833	-1.79115	-0.77989
H	-3.27157	-3.28657	-5.54189	H	6.36053	0.01940	-2.50905
H	-2.65465	-0.88190	-5.20111	H	4.22563	1.27058	-2.90289
H	-1.98156	-0.07207	-2.94314	H	2.19145	0.71145	-1.59169
C	-3.01867	-3.23173	1.46569	C	2.60751	-2.49142	2.98901
C	-3.00790	-4.39377	2.25432	C	3.22567	-2.45255	4.25132
C	-1.84082	-5.16698	2.36112	C	3.65138	-1.23147	4.79397
C	-0.67788	-4.76971	1.68135	C	3.45523	-0.04251	4.07069
C	-0.68351	-3.60425	0.89981	C	2.83229	-0.07590	2.81550
H	-3.93003	-2.62986	1.40062	H	2.28349	-3.45044	2.57413
H	-3.91526	-4.69137	2.79096	H	3.37466	-3.38410	4.80776
H	-1.83532	-6.07148	2.97866	H	4.13252	-1.20394	5.77726
H	0.23998	-5.36118	1.76625	H	3.78238	0.91572	4.48797
H	0.22993	-3.28436	0.38617	H	2.67380	0.85449	2.25911
TS (5-6)_1,2,3,5-C6F4H2_1				C	-4.12916	0.56738	1.85543
SCF (BP86) Energy =				C	-5.04288	-0.48685	2.05788
Enthalpy 0K =				C	-5.70877	-1.11027	0.99091
Enthalpy 298K =				C	-5.48058	-0.62469	-0.31135
Free Energy 298K =				C	-4.57871	0.42019	-0.57988
SCRf (PCM,THF) Energy =				C	-3.53968	1.27330	3.05812
Imaginary Frequency =				H	-5.24656	-0.81322	3.08518
				C	-6.65238	-2.26973	1.22816
Ru	-0.21100	0.27875	0.36173	H	-6.02643	-1.06746	-1.15291
C	-1.53820	1.91981	0.17281	C	-4.41520	0.95536	-1.98256
N	-1.13739	3.22394	-0.06507	C	0.72644	3.95535	-1.51147
C	-2.22494	4.09464	-0.12710	C	2.04900	4.43531	-1.60404
C	-3.34268	3.34393	0.08831	C	2.83900	4.69833	-0.47144
N	-2.91608	2.02866	0.27428	C	2.26522	4.50664	0.79966
C	0.22087	3.70946	-0.21242	C	0.95478	4.02286	0.95715
C	-3.86636	0.96231	0.52425	C	-0.11305	3.76902	-2.75257
H	-4.39463	3.61131	0.13194	H	2.46195	4.62533	-2.60218
H	-2.09431	5.15610	-0.31742	C	4.26788	5.17830	-0.61276
C	-0.40447	0.22571	2.15930	H	2.84727	4.75072	1.69674
O	-0.52903	0.18824	3.33552	C	0.35694	3.86200	2.33669
P	1.62569	-1.25817	0.55753	H	0.50259	3.92601	-3.65309
C	2.40380	-1.30242	2.26262	H	-0.59728	2.76796	-2.81444
C	1.26538	-3.05777	0.22409	H	-0.93083	4.51368	-2.78326
C	3.14631	-0.87311	-0.45730	H	-0.64736	4.31572	2.40076
H	-0.15914	0.62530	-1.62436	H	0.24648	2.79822	2.60748

H	0.99653	4.34150	3.09465
H	4.55582	5.84497	0.21732
H	4.97323	4.32702	-0.60673
H	4.42044	5.72271	-1.55927
H	-5.00101	0.34503	-2.68866
H	-4.79706	1.99148	-2.05032
H	-3.35546	0.98111	-2.32276
H	-7.54644	-2.20180	0.58542
H	-6.15975	-3.23161	0.99624
H	-6.98597	-2.31350	2.27782
H	-2.85076	2.08192	2.77599
H	-4.34933	1.71467	3.66667
H	-2.98477	0.57543	3.70471

TS (2-3) _1,2,3,5-C6F4H2_2

SCF (BP86) Energy = -2464.46241820
Enthalpy 0K = -2463.719183
Enthalpy 298K = -2463.663066
Free Energy 298K = -2463.815516
SCRf (PCM,THF) Energy = -2464.47432794
Lowest frequency = -556.7474 cm-1

Ru	-0.36926	0.16373	-0.28086
C	-1.82893	-1.28606	-0.57345
N	-1.64549	-2.56772	-1.08461
C	-2.85044	-3.27488	-1.15387
C	-3.82615	-2.43874	-0.69968
N	-3.20388	-1.23301	-0.35790
C	-0.42698	-3.09962	-1.66145
C	-3.99026	-0.04415	-0.07975
H	-4.89811	-2.57746	-0.58734
H	-2.89100	-4.29730	-1.51910
C	-1.17969	1.41274	-1.38504
O	-1.66633	2.24779	-2.06801
P	1.54458	1.58170	-0.19979
C	1.53206	2.96020	1.06728
C	3.23173	0.78436	-0.04840
C	1.80841	2.53826	-1.79447
H	0.37354	-0.93785	1.00121
H	0.33745	-0.43705	-1.53006
C	0.14087	-0.92005	2.46738
C	1.32559	-0.56831	3.18661
C	2.01614	-1.43264	4.03349
C	-0.42279	-2.15385	2.90928
C	1.44772	-2.68092	4.31364
C	0.22389	-3.05879	3.74944
F	1.84953	0.65939	2.93273
F	-0.79941	0.17557	2.28486
H	2.95266	-1.11274	4.49439
F	-1.61613	-2.52455	2.35060
F	2.08936	-3.53666	5.15416
H	-0.24085	-4.01873	3.98283
C	-4.35640	0.28827	1.24456
C	-5.14559	1.43947	1.43592
C	-5.58584	2.23734	0.36664
C	-5.25368	1.83451	-0.93939
C	-4.47233	0.69399	-1.19013
C	-3.96129	-0.55491	2.43313
H	-5.43161	1.70880	2.45995
C	-6.39507	3.49316	0.61013
H	-5.61700	2.41860	-1.79325
C	-4.20920	0.25248	-2.61253
H	-3.13927	0.07070	-2.79500
H	-4.74421	-0.68681	-2.84391
H	-4.54853	1.02005	-3.32484
H	-4.57292	-0.28732	3.30967
H	-4.09176	-1.63047	2.23397
H	-2.90241	-0.40442	2.69063
H	-6.91813	3.45658	1.57988

H	-5.74448	4.38696	0.62092
H	-7.14740	3.65055	-0.18097
C	0.32622	-4.06622	-0.96032
C	1.49233	-4.56741	-1.57394
C	1.90168	-4.15861	-2.85233
C	1.08804	-3.24083	-3.54479
C	-0.08078	-2.70512	-2.98008
C	-0.10330	-4.61922	0.37933
H	2.08986	-5.30926	-1.02987
C	3.17899	-4.68374	-3.47198
H	1.36387	-2.93925	-4.56270
C	-0.94687	-1.75949	-3.78078
H	-0.80546	-3.95593	0.89939
H	-0.59865	-5.60027	0.25161
H	0.76862	-4.78263	1.03346
H	-0.89410	-0.73509	-3.37327
H	-0.62092	-1.73122	-4.83264
H	-2.00743	-2.06471	-3.75785
H	3.49066	-5.63594	-3.01241
H	3.06529	-4.84722	-4.55706
H	4.00845	-3.96551	-3.33735
C	3.32824	-0.54798	0.39705
C	4.58139	-1.17221	0.50821
C	5.75071	-0.47266	0.17165
C	5.66272	0.85134	-0.29045
C	4.41077	1.47485	-0.40756
H	2.41101	-1.09579	0.63566
H	4.64047	-2.20931	0.85513
H	6.72796	-0.95984	0.25786
H	6.56964	1.39821	-0.57029
H	4.34822	2.49583	-0.79868
C	1.91939	3.94128	-1.84050
C	2.11564	4.59906	-3.06803
C	2.21043	3.86343	-4.25803
C	2.10446	2.46222	-4.21888
C	1.90047	1.80484	-2.99773
H	1.84976	4.52571	-0.91822
H	2.19435	5.69145	-3.08853
H	2.36319	4.37734	-5.21302
H	2.17524	1.87944	-5.14374
H	1.80503	0.71375	-2.97380
C	2.67799	3.45064	1.72437
C	2.56799	4.49600	2.65576
C	1.31576	5.06486	2.93835
C	0.16853	4.57855	2.29068
C	0.27486	3.52823	1.36604
H	3.65752	3.00701	1.52237
H	3.46570	4.86326	3.16494
H	1.23339	5.87892	3.66636
H	-0.81395	5.00939	2.51109
H	-0.62355	3.13691	0.87569

TS (5-6) _1,2,3,5-C6F4H2_2

SCF (BP86) Energy = -2464.45465828
Enthalpy 0K = -2463.709201
Enthalpy 298K = -2463.653067
Free Energy 298K = -2463.804602
SCRf (PCM,THF) Energy = -2464.47452530
Imaginary Frequency = -344.6802 cm-1

Ru	0.28584	0.12859	0.04960
C	1.67483	1.64593	-0.26127
N	1.35284	2.98122	-0.45110
C	2.48581	3.74852	-0.73738
C	3.54693	2.89487	-0.74635
N	3.04603	1.61812	-0.46426
C	0.02339	3.56391	-0.49801
C	3.90902	0.45869	-0.55882
H	4.60517	3.05950	-0.92850

H	2.41657	4.82042	-0.89987
C	1.41394	-1.26575	-0.08266
O	2.08335	-2.24230	-0.09885
P	-1.49222	-1.43502	-0.47824
C	-1.08626	-2.49049	-1.98380
C	-2.04592	-2.73848	0.74028
C	-3.07767	-0.62955	-1.04701
H	-0.85503	1.60681	1.47113
H	0.18155	0.26350	-1.53428
C	-0.55974	0.81045	2.19043
C	0.79098	0.59086	2.58143
C	1.17215	-0.45041	3.46822
C	-1.49646	-0.14931	2.68474
C	0.18882	-1.31332	3.91850
C	-1.16838	-1.17329	3.55014
F	1.67491	1.64096	2.48938
F	-1.26510	2.36226	3.19592
H	2.20720	-0.54002	3.80144
F	-2.78863	0.00212	2.30182
F	0.52447	-2.34249	4.74066
H	-1.92604	-1.87254	3.90635
C	-3.38549	-2.89148	1.14704
C	-3.72993	-3.87530	2.08996
C	-2.74484	-4.71855	2.62732
C	-1.40568	-4.56818	2.22810
C	-1.05468	-3.57655	1.30029
H	-4.16141	-2.24113	0.73410
H	-4.77444	-3.98109	2.40190
H	-3.01727	-5.48618	3.35922
H	-0.62805	-5.21256	2.65078
H	-0.00562	-3.45507	1.01063
C	-4.01327	-1.33928	-1.83196
C	-5.20239	-0.72142	-2.24679
C	-5.46619	0.61200	-1.88958
C	-4.53526	1.32592	-1.12004
C	-3.34500	0.70937	-0.70111
H	-3.80778	-2.37436	-2.12372
H	-5.92179	-1.28203	-2.85313
H	-6.39436	1.09339	-2.21552
H	-4.72754	2.36610	-0.84025
H	-2.62752	1.27972	-0.10421
C	-1.27595	-3.88727	-2.00443
C	-0.99853	-4.62844	-3.16655
C	-0.54173	-3.98528	-4.32557
C	-0.36234	-2.59185	-4.31812
C	-0.62827	-1.85268	-3.15683
H	-1.63808	-4.40467	-1.11207
H	-1.14446	-5.71388	-3.15977
H	-0.32689	-4.56406	-5.23003
H	-0.01022	-2.07701	-5.21844
H	-0.47628	-0.76842	-3.15680
C	3.98171	-0.22117	-1.79852
C	4.86607	-1.30790	-1.90224
C	5.67202	-1.71813	-0.82500
C	5.60373	-0.98522	0.37267
C	4.74157	0.11556	0.53077
C	3.14413	0.20338	-2.98291
H	4.92351	-1.84888	-2.85436
C	6.57759	-2.92422	-0.94866
H	6.24606	-1.27083	1.21441
C	4.75568	0.91824	1.81162
C	-0.45883	4.30173	0.61122
C	-1.73026	4.90096	0.48118
C	-2.48495	4.82480	-0.69898
C	-1.93933	4.13138	-1.79768
C	-0.68152	3.51059	-1.73049
C	0.28560	4.43698	1.91168
H	-2.12934	5.44936	1.34235

C	-3.82564	5.52147	-0.80770
H	-2.49648	4.08964	-2.74118
C	-0.08922	2.86120	-2.96115
H	5.26146	1.89119	1.66772
H	3.73980	1.13803	2.17027
H	5.30329	0.37838	2.60040
H	7.44552	-2.85143	-0.27275
H	6.03449	-3.85080	-0.68695
H	6.95219	-3.04629	-1.97867
H	3.43183	-0.36116	-3.88363
H	2.07113	0.02760	-2.79124
H	3.26059	1.28012	-3.19874
H	0.15615	5.45420	2.31839
H	-0.16795	3.70634	2.62939
H	1.36060	4.22940	1.81130
H	0.90770	3.27527	-3.19545
H	0.04094	1.77387	-2.81950
H	-0.74054	3.02188	-3.83471
H	-4.45221	5.07568	-1.59798
H	-4.38238	5.47532	0.14299
H	-3.69888	6.59130	-1.05723

TS (2-3)_1,2,3,5-C6F4H2_5

SCF (BP86) Energy =	-2464.45706612		
Enthalpy 0K =	-2463.713893		
Enthalpy 298K =	-2463.657700		
Free Energy 298K =	-2463.810519		
SCRF (PCM,THF) Energy =	-2464.47004664		
Lowest frequency =	-592.2865 cm-1		
Ru	-0.40878	0.27944	-0.39502
C	-1.91638	-1.09988	-0.77011
N	-1.78220	-2.31541	-1.43366
C	-3.00152	-2.99534	-1.52388
C	-3.93819	-2.20905	-0.92164
N	-3.27637	-1.06244	-0.46842
C	-0.60661	-2.79911	-2.13074
C	-4.02095	0.08411	0.01927
H	-5.00562	-2.34695	-0.77125
H	-3.07902	-3.96374	-2.01074
C	-1.21871	1.67613	-1.30428
O	-1.70730	2.60836	-1.84570
P	1.57507	1.56982	-0.19845
C	1.72221	2.63738	1.33356
C	3.20010	0.64182	-0.25487
C	1.84739	2.81383	-1.57225
H	0.32943	-0.94052	0.75858
H	0.21622	-0.19596	-1.74563
C	0.07550	-0.96047	2.20656
C	1.25775	-0.62130	2.93440
C	1.82695	-1.55344	3.79742
C	-0.58994	-2.17990	2.54446
C	1.23401	-2.80006	4.06103
C	0.01898	-3.07998	3.41697
H	1.74203	0.34671	2.79766
F	-0.84303	0.19243	2.03069
F	2.98063	-1.25051	4.44087
H	-1.53366	-2.45078	2.07120
F	1.81315	-3.69571	4.89639
F	-0.58027	-4.27194	3.66586
C	-4.32438	0.21063	1.39349
C	-5.07460	1.33191	1.79838
C	-5.53379	2.29738	0.88694
C	-5.26518	2.09873	-0.47982
C	-4.52773	0.99530	-0.94091
C	-3.89538	-0.81173	2.41950
H	-5.31205	1.44248	2.86339
C	-6.29757	3.51607	1.35870
H	-5.64766	2.81712	-1.21456

C	-4.34775	0.76791	-2.42540
H	-3.30612	0.52509	-2.68351
H	-4.97632	-0.07178	-2.77550
H	-4.63727	1.66553	-2.99277
H	-4.54684	-0.76379	3.30685
H	-3.93726	-1.83855	2.01960
H	-2.85954	-0.62705	2.74605
H	-6.78080	3.33926	2.33360
H	-5.62249	4.38328	1.47868
H	-7.07728	3.81072	0.63638
C	0.19007	-3.80518	-1.54049
C	1.28949	-4.28837	-2.27456
C	1.60181	-3.80879	-3.55863
C	0.75918	-2.83522	-4.12544
C	-0.35483	-2.32055	-3.43891
C	-0.11711	-4.36055	-0.17059
H	1.91522	-5.06897	-1.82522
C	2.81463	-4.31854	-4.30722
H	0.96496	-2.46971	-5.13887
C	-1.25070	-1.29502	-4.09500
H	-1.15116	-4.74127	-0.10040
H	0.56528	-5.18866	0.07719
H	-0.01177	-3.58666	0.60874
H	-1.15527	-0.31642	-3.59251
H	-0.98543	-1.16760	-5.15643
H	-2.31406	-1.58655	-4.03964
H	3.07288	-5.34769	-4.00761
H	2.65154	-4.30867	-5.39780
H	3.69857	-3.68658	-4.10377
C	3.21958	-0.73204	0.05648
C	4.42799	-1.44731	0.03641
C	5.62622	-0.79961	-0.30229
C	5.61348	0.56726	-0.62698
C	4.40742	1.28515	-0.60650
H	2.27722	-1.23509	0.29728
H	4.42955	-2.51433	0.28248
H	6.56774	-1.35894	-0.32048
H	6.54319	1.07634	-0.90309
H	4.40244	2.34591	-0.87834
C	2.19902	4.15659	-1.33143
C	2.40579	5.03932	-2.40609
C	2.27128	4.58843	-3.72752
C	1.92314	3.24929	-3.97402
C	1.70707	2.36884	-2.90455
H	2.30839	4.51755	-0.30419
H	2.67286	6.08238	-2.20488
H	2.43193	5.27773	-4.56322
H	1.81016	2.89096	-5.00287
H	1.41608	1.33064	-3.09733
C	2.91605	2.81745	2.06260
C	2.92716	3.61971	3.21668
C	1.75206	4.25452	3.64848
C	0.55893	4.07963	2.92720
C	0.54112	3.26902	1.78273
H	3.83701	2.32479	1.73542
H	3.85842	3.74466	3.77944
H	1.76336	4.87680	4.54951
H	-0.36399	4.56406	3.26310
H	-0.39519	3.11130	1.23598
TS(5-6)_1,2,3,5-C6F4H2_5			
SCF (BP86) Energy = -2464.46580869			
Enthalpy 0K = -2463.719131			
Enthalpy 298K = -2463.663413			
Free Energy 298K = -2463.814859			
SCRf (PCM,THF) Energy = -2464.48151922			
Imaginary Frequency = -224.2770 cm-1			
Ru	0.09848	-0.38035	0.35060

C	1.23021	-2.16429	0.11378
N	0.66607	-3.39205	-0.19725
C	1.62273	-4.40508	-0.25013
C	2.82298	-3.82634	0.03734
N	2.57562	-2.47024	0.25768
C	-0.73254	-3.67824	-0.44865
C	3.67215	-1.56246	0.53739
H	3.82569	-4.23841	0.10809
H	1.35385	-5.43057	-0.48729
C	0.17725	-0.47545	2.15769
O	0.22667	-0.53607	3.33970
P	-1.56441	1.32701	0.53930
C	-2.52792	1.30619	2.14743
C	-0.96901	3.09091	0.43880
C	-2.99058	1.21495	-0.66640
H	0.11301	-0.52415	-1.62026
H	-1.12927	-1.35974	0.44277
C	0.67392	0.44014	-1.85697
C	1.73062	0.91189	-1.02240
C	2.18446	2.23603	-1.17368
C	0.01542	1.35509	-2.72522
C	1.61892	3.10775	-2.10192
C	0.53746	2.63332	-2.87650
H	2.37814	0.23171	-0.45925
F	1.38131	-1.04934	-2.93337
F	3.22115	2.67196	-0.42025
H	-0.85031	1.05710	-3.31764
F	2.07791	4.37026	-2.26191
F	-0.03553	3.50174	-3.74212
C	-1.43192	4.03030	-0.50343
C	-0.88635	5.32489	-0.53903
C	0.11962	5.69498	0.36588
C	0.59059	4.76189	1.30496
C	0.05868	3.46476	1.33417
H	-2.20860	3.75189	-1.22107
H	-1.24606	6.04098	-1.28505
H	0.54538	6.70304	0.33228
H	1.38491	5.03768	2.00621
H	0.44944	2.73353	2.05057
C	-4.09284	2.09261	-0.56718
C	-5.17624	1.97442	-1.45069
C	-5.17924	0.96958	-2.43298
C	-4.09921	0.07798	-2.52141
C	-3.01085	0.19854	-1.64129
H	-4.11071	2.86220	0.21162
H	-6.02290	2.66385	-1.36581
H	-6.02694	0.87672	-3.12003
H	-4.09972	-0.71838	-3.27268
H	-2.18277	-0.51468	-1.69861
C	-2.76150	2.46200	2.91795
C	-3.52779	2.38604	4.09401
C	-4.07302	1.16106	4.50568
C	-3.84782	0.00608	3.73759
C	-3.07717	0.07586	2.56848
H	-2.34207	3.42312	2.60600
H	-3.69715	3.29113	4.68710
H	-4.66890	1.10419	5.42264
H	-4.26703	-0.95503	4.05366
H	-2.89499	-0.82891	1.97818
C	3.99046	-1.24821	1.87788
C	5.06496	-0.36520	2.10485
C	5.82488	0.17062	1.05245
C	5.52358	-0.23664	-0.26121
C	4.46530	-1.11536	-0.55397
C	3.26434	-1.85645	3.05816
H	5.31951	-0.10566	3.13973
C	6.94398	1.15412	1.31863
H	6.13604	0.13307	-1.09208

C	4.21309	-1.57261	-1.97126
C	-1.18258	-3.76037	-1.78813
C	-2.54614	-4.05807	-1.98896
C	-3.43174	-4.29894	-0.92394
C	-2.91929	-4.27467	0.38714
C	-1.57103	-3.97747	0.65189
C	-0.24960	-3.58851	-2.96278
H	-2.91625	-4.12317	-3.01944
C	-4.89721	-4.58176	-1.17797
H	-3.58244	-4.50529	1.22981
C	-1.04380	-3.99110	2.06878
H	-0.81203	-3.66883	-3.90729
H	0.30397	-2.62143	-2.95499
H	0.51861	-4.38411	-2.97095
H	-0.12260	-4.59320	2.15501
H	-0.79465	-2.97411	2.41639
H	-1.79253	-4.41330	2.75763
H	-5.31120	-5.27872	-0.43012
H	-5.49478	-3.65323	-1.12338
H	-5.05822	-5.01641	-2.17828
H	4.93687	-1.09813	-2.65324
H	4.34412	-2.66699	-2.06052
H	3.18405	-1.34296	-2.32941
H	7.80560	0.97716	0.65298
H	6.60494	2.19100	1.14102
H	7.29657	1.09579	2.36140
H	2.73310	-2.78146	2.78587
H	3.98326	-2.09708	3.85931
H	2.51793	-1.16578	3.48249

TS (2-3)_1,2,3-C6F3H3_1

SCF (BP86) Energy =	-2365.22798744
Enthalpy 0K =	-2364.476744
Enthalpy 298K =	-2364.421567
Free Energy 298K =	-2364.571961
SCRf (PCM,THF) Energy =	-2365.24148045
Imaginary Frequency =	-600.7069 cm ⁻¹
Ru	0.38325 -0.01473 -0.26121
C	1.92718 1.36858 -0.14056
N	1.81073 2.75080 -0.25670
C	3.05179 3.38812 -0.15103
C	3.98497 2.41022 0.02490
N	3.30014 1.18955 0.02892
C	0.62324 3.49168 -0.63507
C	4.02151 -0.06817 -0.04570
H	5.06417 2.45765 0.14397
H	3.14479 4.46873 -0.21855
C	1.07984 -0.90690 -1.72868
O	1.49765 -1.52266 -2.64929
P	-1.63385 -1.24781 -0.55549
C	-1.70460 -2.96930 0.17613
C	-3.24347 -0.43590 -0.05133
C	-2.01475 -1.59027 -2.36255
H	-0.22278 0.65840 1.33230
H	-0.29629 0.99495 -1.23617
C	0.15980 0.11921 2.67589
C	-1.00071 -0.41172 3.31234
C	-1.51319 0.15458 4.48093
C	0.89160 1.09094 3.42669
C	-0.83496 1.17133 5.16598
C	0.37721 1.62178 4.61540
F	-1.68162 -1.41635 2.70425
F	0.97104 -0.90261 2.00538
F	-2.67174 -0.34862 4.97574
H	1.83017 1.46258 3.01211
H	-1.24835 1.57040 6.09434
H	0.94719 2.39925 5.13475
C	4.40174 -0.75078 1.13172

C	5.12120	-1.95345	0.98985
C	5.47956	-2.47079	-0.26604
C	5.14188	-1.72443	-1.40987
C	4.43109	-0.51530	-1.32724
C	4.08966	-0.22757	2.51402
H	5.41627	-2.49372	1.89756
C	6.21077	-3.79044	-0.38778
H	5.44781	-2.08533	-2.39900
C	4.18175	0.30483	-2.57334
H	3.14026	0.65253	-2.63902
H	4.82885	1.20136	-2.59129
H	4.39875	-0.28632	-3.47602
H	4.79350	-0.64605	3.25139
H	4.15782	0.87206	2.56126
H	3.06904	-0.50769	2.81915
H	6.75825	-4.03730	0.53665
H	5.50326	-4.61748	-0.58167
H	6.93171	-3.77920	-1.22243
C	-0.10697	4.19226	0.35015
C	-1.22214	4.94318	-0.06627
C	-1.61289	5.01882	-1.41450
C	-0.83356	4.33997	-2.36886
C	0.29231	3.57812	-2.00886
C	0.28649	4.15408	1.80688
H	-1.79722	5.48880	0.69162
C	-2.84102	5.80145	-1.82733
H	-1.09959	4.41209	-3.43050
C	1.11606	2.88480	-3.06952
H	1.33791	4.45654	1.95780
H	-0.34913	4.83081	2.39957
H	0.18645	3.13868	2.22657
H	0.99105	1.78967	-3.00507
H	0.80871	3.20947	-4.07618
H	2.19309	3.09729	-2.95395
H	-3.04391	6.63344	-1.13283
H	-2.73324	6.21931	-2.84215
H	-3.73769	5.15486	-1.83410
C	-3.22222	0.64003	0.85697
C	-4.41730	1.26634	1.24595
C	-5.64566	0.82669	0.72857
C	-5.67513	-0.23579	-0.19011
C	-4.48130	-0.86016	-0.58373
H	-2.25962	0.99296	1.24027
H	-4.38528	2.10146	1.95369
H	-6.57762	1.31544	1.03243
H	-6.62865	-0.57552	-0.60875
H	-4.51039	-1.66926	-1.32110
C	-2.26238	-2.88326	-2.86286
C	-2.54315	-3.07633	-4.22734
C	-2.58736	-1.98165	-5.10257
C	-2.34518	-0.68778	-4.60926
C	-2.05630	-0.49361	-3.25131
H	-2.23347	-3.74467	-2.18894
H	-2.72766	-4.08885	-4.60248
H	-2.80625	-2.13374	-6.16486
H	-2.37556	0.17311	-5.28603
H	-1.85312	0.51467	-2.87429
C	-2.87247	-3.56441	0.69307
C	-2.83168	-4.86728	1.21579
C	-1.62796	-5.58999	1.22455
C	-0.45905	-5.00155	0.71498
C	-0.49519	-3.69652	0.20040
H	-3.81336	-3.00608	0.70359
H	-3.74476	-5.31552	1.62229
H	-1.59922	-6.60505	1.63485
H	0.48674	-5.55372	0.72655
H	0.42150	-3.23100	-0.17811

TS (5-6)_1,2,3-C6F3H3_1

SCF (BP86) Energy = -2365.23621870
Enthalpy 0K = -2364.481921
Enthalpy 298K = -2364.427103
Free Energy 298K = -2364.576227
SCRF (PCM,THF) Energy = -2365.25194686
Imaginary Frequency = -190.5167 cm-1
Ru -0.28108 0.18717 0.33271
C -1.79503 1.65408 0.15463
N -1.56147 3.00327 -0.05002
C -2.75166 3.72623 -0.12919
C -3.76714 2.83295 0.04448
N -3.17728 1.58106 0.22263
C -0.27445 3.66577 -0.13361
C -3.98285 0.39857 0.45602
H -4.84568 2.96107 0.06350
H -2.75607 4.79909 -0.29920
C -0.51799 0.03794 2.12046
O -0.66800 -0.06056 3.29066
P 1.70265 -1.15135 0.54442
C 2.49313 -1.07430 2.24397
C 1.49705 -2.98478 0.26987
C 3.18143 -0.66905 -0.49053
H -0.15735 0.60225 -1.61606
H 0.67781 1.39284 0.64855
C -0.52189 -0.38722 -2.05099
C -1.35242 -1.30317 -1.34080
C -1.44745 -2.65422 -1.73856
C 0.30394 -0.92365 -3.06976
C -0.70549 -3.13819 -2.81806
C 0.16458 -2.24879 -3.47674
H -2.09469 -0.92006 -0.61990
F -1.64551 0.96954 -2.84741
H -2.13584 -3.31721 -1.20681
F 1.18464 -0.11234 -3.71416
H -0.78007 -4.16964 -3.16901
F 0.92334 -2.69259 -4.50920
C 2.21109 -3.71597 -0.69884
C 1.97218 -5.09102 -0.86643
C 1.02375 -5.74813 -0.06902
C 0.29819 -5.02219 0.89144
C 0.52372 -3.64768 1.05147
H 2.95206 -3.21551 -1.32852
H 2.53216 -5.64638 -1.62624
H 0.84372 -6.82055 -0.19871
H -0.45099 -5.52482 1.51248
H -0.05942 -3.08309 1.78753
C 4.42826 -1.30874 -0.30464
C 5.54684 -0.90958 -1.04941
C 5.43743 0.14027 -1.97818
C 4.20773 0.79077 -2.15391
C 3.08403 0.39050 -1.41125
H 4.52705 -2.11138 0.43367
H 6.50717 -1.41416 -0.89896
H 6.31252 0.45240 -2.55797
H 4.11408 1.61227 -2.87111
H 2.13240 0.90940 -1.54759
C 2.89831 -2.21797 2.95943
C 3.52757 -2.08567 4.20957
C 3.76510 -0.81403 4.75151
C 3.36849 0.33052 4.03925
C 2.73319 0.20259 2.79605
H 2.72064 -3.21529 2.54620
H 3.83284 -2.98350 4.75767
H 4.25495 -0.71345 5.72573
H 3.54757 1.32734 4.45602
H 2.41608 1.09736 2.24920
C -4.21338 -0.02714 1.78407

C -4.98539 -1.19086 1.97552
C -5.54959 -1.89535 0.89993
C -5.36314 -1.38647 -0.40014
C -4.59907 -0.23358 -0.65720
C -3.74522 0.75449 2.99330
H -5.16137 -1.53978 3.00054
C -6.34478 -3.16351 1.12784
H -5.83603 -1.89459 -1.24912
C -4.48763 0.32022 -2.05759
C 0.23977 4.01711 -1.40426
C 1.48856 4.67137 -1.43265
C 2.19594 5.00119 -0.26376
C 1.60965 4.69245 0.97847
C 0.37129 4.03409 1.07164
C -0.52153 3.75716 -2.68201
H 1.90783 4.94460 -2.40858
C 3.55048 5.67373 -0.33546
H 2.12254 4.98163 1.90394
C -0.24515 3.74806 2.42243
H 0.10767 3.99738 -3.55431
H -0.88420 2.70916 -2.77208
H -1.41743 4.40410 -2.73877
H -1.30419 4.05734 2.46055
H -0.21583 2.67076 2.65902
H 0.29578 4.28594 3.21718
H 3.69984 6.37487 0.50287
H 4.36597 4.92894 -0.28553
H 3.67523 6.23315 -1.27715
H -4.95005 -0.37494 -2.77663
H -5.02924 1.28183 -2.13714
H -3.43797 0.51575 -2.36874
H -7.20641 -3.22901 0.44226
H -5.72246 -4.06009 0.95123
H -6.72267 -3.22481 2.16155
H -3.07943 1.58680 2.72635
H -4.61651 1.17651 3.52665
H -3.20406 0.10972 3.70324

TS (2-3)_1,2,3-C6F3H3_2

SCF (BP86) Energy = -2365.23247244
Enthalpy 0K = -2364.481181
Enthalpy 298K = -2364.426011
Free Energy 298K = -2364.576023
SCRF (PCM,THF) Energy = -2365.24496481
Lowest frequency = -572.4426 cm-1
Ru 0.30843 -0.08965 -0.21704
C 1.89012 1.24995 -0.35882
N 1.81079 2.61300 -0.62889
C 3.07573 3.20940 -0.65925
C 3.98432 2.22124 -0.42388
N 3.26203 1.03528 -0.25187
C 0.62394 3.34624 -1.02121
C 3.93799 -0.24989 -0.23444
H 5.06920 2.24037 -0.36351
H 3.20020 4.27254 -0.84533
C 0.92827 -1.18844 -1.57617
O 1.28956 -1.92505 -2.42916
P -1.72844 -1.32738 -0.24655
C -1.78230 -2.90603 0.75889
C -3.32070 -0.42766 0.15426
C -2.16912 -1.95905 -1.96007
H -0.25453 0.83837 1.26617
H -0.40218 0.78760 -1.28802
C 0.05296 0.53100 2.70198
C -1.13100 0.17057 3.41706
C -1.69173 0.94613 4.42720
C 0.75326 1.61997 3.30103
C -1.00910 2.08441 4.89214

C	0.22579	2.42060	4.31000
F	-1.77845	-0.94976	2.99364
F	0.86605	-0.59010	2.27176
H	-2.63867	0.61856	4.86508
F	1.95528	1.96560	2.73844
H	-1.42531	2.69062	5.70035
H	0.81153	3.27905	4.65076
C	4.33574	-0.84187	0.98609
C	5.01356	-2.07543	0.92475
C	5.31672	-2.70877	-0.29207
C	4.96160	-2.05354	-1.48494
C	4.28708	-0.82098	-1.48439
C	4.08946	-0.18827	2.32465
H	5.32249	-2.54566	1.86625
C	6.00672	-4.05572	-0.32151
H	5.22127	-2.50812	-2.44837
C	3.99783	-0.11420	-2.78988
H	2.93922	0.17430	-2.87493
H	4.59698	0.80983	-2.88501
H	4.24048	-0.76514	-3.64380
H	4.71294	-0.66206	3.09977
H	4.32027	0.88865	2.30333
H	3.03489	-0.28117	2.62337
H	6.57920	-4.23815	0.60281
H	5.27089	-4.87498	-0.41966
H	6.69842	-4.13840	-1.17670
C	0.00846	4.23640	-0.11482
C	-1.13099	4.94175	-0.55313
C	-1.64425	4.80458	-1.85170
C	-0.96399	3.95396	-2.74494
C	0.17236	3.22384	-2.36123
C	0.55619	4.49916	1.26932
H	-1.62264	5.62576	0.14965
C	-2.89212	5.54426	-2.28420
H	-1.32096	3.86310	-3.77815
C	0.89595	2.35939	-3.36847
H	1.23516	3.70665	1.60762
H	1.11405	5.45442	1.28884
H	-0.26116	4.58844	2.00341
H	0.76274	1.28856	-3.13659
H	0.51323	2.54435	-4.38474
H	1.98149	2.55969	-3.36835
H	-3.08747	6.41908	-1.64263
H	-2.81430	5.89437	-3.32753
H	-3.78041	4.88874	-2.22765
C	-3.26427	0.80913	0.82503
C	-4.44363	1.51071	1.12388
C	-5.69108	0.98516	0.75299
C	-5.75597	-0.24050	0.06898
C	-4.57808	-0.93994	-0.23621
H	-2.28751	1.22427	1.09300
H	-4.38339	2.47214	1.64486
H	-6.61076	1.53287	0.98565
H	-6.72487	-0.64939	-0.23756
H	-4.63523	-1.87817	-0.79817
C	-2.42692	-3.31532	-2.23777
C	-2.75332	-3.72437	-3.54321
C	-2.83292	-2.78419	-4.58051
C	-2.58051	-1.42807	-4.30967
C	-2.24667	-1.01912	-3.01111
H	-2.37074	-4.05770	-1.43607
H	-2.94556	-4.78382	-3.74471
H	-3.08721	-3.10454	-5.59648
H	-2.63800	-0.68678	-5.11416
H	-2.03707	0.03668	-2.80752
C	-2.93372	-3.40414	1.40030
C	-2.87694	-4.60453	2.12702
C	-1.67317	-5.32155	2.21859

C	-0.52024	-4.82906	1.58590
C	-0.57260	-3.62542	0.86623
H	-3.87409	-2.84739	1.34763
H	-3.77763	-4.97710	2.62701
H	-1.63200	-6.25652	2.78749
H	0.42578	-5.37602	1.65934
H	0.33249	-3.23247	0.38961

TS (5-6)_1,2,3-C6F3H3_2

SCF (BP86) Energy =	-2365.22206403		
Enthalpy 0K =	-2364.468645		
Enthalpy 298K =	-2364.413400		
Free Energy 298K =	-2364.563791		
SCRF (PCM,THF) Energy =	-2365.24271222		
Imaginary Frequency =	-348.8769 cm-1		
Ru	0.29625	0.07849	0.14179
C	1.71358	1.54593	-0.25968
N	1.41374	2.87182	-0.53593
C	2.55898	3.60007	-0.87055
C	3.60597	2.73037	-0.82412
N	3.08431	1.48281	-0.46068
C	0.09363	3.47007	-0.63184
C	3.92894	0.30646	-0.48324
H	4.66663	2.86552	-1.01611
H	2.50742	4.66026	-1.10191
C	1.38572	-1.34934	0.04008
O	2.02847	-2.34407	0.05126
P	-1.53561	-1.45382	-0.28750
C	-1.17793	-2.54881	-1.77719
C	-2.08789	-2.71768	0.97365
C	-3.11712	-0.63549	-0.84945
H	-0.79206	1.61737	1.50051
H	0.16382	0.13943	-1.43903
C	-0.48582	0.86939	2.26922
C	0.86180	0.71017	2.69527
C	1.25357	-0.26872	3.63754
C	-1.40332	-0.07632	2.81815
C	0.30003	-1.14332	4.15071
C	-1.05337	-1.03946	3.74592
F	1.73767	1.74987	2.49266
F	-1.21406	2.51484	3.11670
H	2.29494	-0.29085	3.96839
F	-2.69963	0.02895	2.42180
H	0.59227	-1.91138	4.87250
H	-1.82253	-1.71245	4.13127
C	-3.42768	-2.85997	1.38401
C	-3.77392	-3.82094	2.34893
C	-2.79035	-4.65398	2.90492
C	-1.45101	-4.51268	2.50422
C	-1.09747	-3.54063	1.55623
H	-4.20250	-2.21792	0.95633
H	-4.81858	-3.91761	2.66328
H	-3.06468	-5.40620	3.65210
H	-0.67449	-5.15044	2.93955
H	-0.04773	-3.42422	1.26756
C	-4.07482	-1.34961	-1.60359
C	-5.26258	-0.72535	-2.01268
C	-5.50304	0.61898	-1.68070
C	-4.55026	1.33691	-0.94228
C	-3.36115	0.71418	-0.52904
H	-3.88789	-2.39371	-1.87498
H	-5.99935	-1.28971	-2.59422
H	-6.43042	1.10533	-2.00157
H	-4.72509	2.38496	-0.68103
H	-2.62841	1.28691	0.04603
C	-1.28140	-3.95336	-1.73759
C	-1.02473	-4.72087	-2.88771
C	-0.67631	-4.09687	-4.09362

C	-0.58495	-2.69551	-4.14605	C	-2.06867	-2.11182	-1.96519
C	-0.82922	-1.92976	-2.99757	H	-0.22487	0.83994	1.18764
H	-1.56143	-4.45674	-0.80842	H	-0.39527	0.69155	-1.41684
H	-1.10262	-5.81203	-2.83428	C	0.21509	0.58296	2.56837
H	-0.47869	-4.69607	-4.98866	C	-0.89830	0.16475	3.36146
H	-0.32023	-2.19543	-5.08390	C	-1.37026	0.88067	4.45676
H	-0.74964	-0.83882	-3.04734	C	0.96322	1.67202	3.10871
C	3.98514	-0.45423	-1.67607	C	-0.64653	2.00266	4.88609
C	4.85526	-1.55668	-1.71307	C	0.51987	2.39715	4.22530
C	5.66226	-1.90646	-0.61558	F	-1.57491	-0.94531	2.96056
C	5.61026	-1.09645	0.53215	F	1.02980	-0.54343	2.06107
C	4.76372	0.02407	0.62198	H	-2.26339	0.54065	4.98589
C	3.14314	-0.10086	-2.88059	H	1.87195	1.97953	2.58796
H	4.89956	-2.15963	-2.62794	F	-1.08623	2.70133	5.97029
C	6.55186	-3.12973	-0.66537	H	1.08800	3.25675	4.59122
H	6.25428	-1.33462	1.38732	C	4.43367	-0.47523	1.03569
C	4.79942	0.91079	1.84577	C	5.19158	-1.66203	1.06983
C	-0.38688	4.28472	0.42211	C	5.52492	-2.37452	-0.09406
C	-1.64789	4.89404	0.23984	C	5.11953	-1.84492	-1.33274
C	-2.39173	4.75458	-0.94066	C	4.36803	-0.66151	-1.42667
C	-1.84618	3.98432	-1.98770	C	4.14854	0.26404	2.32172
C	-0.59970	3.35060	-1.86697	H	5.53742	-2.03086	2.04311
C	0.34779	4.49340	1.71774	C	6.29975	-3.67269	-0.02065
H	-2.04639	5.50308	1.05954	H	5.40274	-2.36005	-2.25829
C	-3.71912	5.46392	-1.11185	C	4.04193	-0.07561	-2.78229
H	-2.39435	3.89128	-2.93286	H	2.98568	0.22126	-2.86133
C	-0.00169	2.62074	-3.04880	H	4.65161	0.82554	-2.97988
H	5.33698	1.85489	1.63824	H	4.24934	-0.80524	-3.57980
H	3.79039	1.18655	2.18431	H	4.88543	-0.00933	3.09402
H	5.32829	0.40891	2.67165	H	4.18754	1.35747	2.18349
H	7.42201	-3.02665	0.00376	H	3.14533	0.01532	2.70277
H	5.99743	-4.03145	-0.34667	H	6.88909	-3.74106	0.90848
H	6.92297	-3.31999	-1.68628	H	5.61691	-4.54185	-0.04161
H	3.43258	-0.71341	-3.74884	H	6.98917	-3.78237	-0.87458
H	2.07138	-0.27279	-2.67824	C	-0.26720	4.13745	-0.41216
H	3.25261	0.96271	-3.15631	C	-1.41873	4.77451	-0.91130
H	0.21985	5.53343	2.06253	C	-1.85588	4.60085	-2.23597
H	-0.11485	3.80725	2.47389	C	-1.08709	3.78416	-3.08510
H	1.42255	4.27555	1.63782	C	0.07383	3.12713	-2.64008
H	0.98855	3.03128	-3.31642	C	0.17395	4.36744	1.01297
H	0.14560	1.54897	-2.82899	H	-1.98539	5.43071	-0.23967
H	-0.65691	2.70861	-3.92982	C	-3.12124	5.26659	-2.73283
H	-4.39123	4.90936	-1.78801	H	-1.39007	3.66082	-4.13201
H	-4.23294	5.59738	-0.14575	C	0.88454	2.28015	-3.59375
H	-3.57915	6.47023	-1.54876	H	1.21985	4.71746	1.06955
TS (2-3)_1,2,4-C6F3H3_1				H	-0.46264	5.12235	1.50087
SCF (BP86) Energy =				H	0.11866	3.44034	1.60815
Enthalpy 0K =				H	0.80216	1.21095	-3.33082
Enthalpy 298K =				H	0.53038	2.41052	-4.62856
Free Energy 298K =				H	1.95642	2.54205	-3.56208
SCRf (PCM,THF) Energy =				H	-3.33047	6.19982	-2.18423
Lowest frequency =				H	-3.05822	5.50626	-3.80740
Ru 0.34470 -0.09898 -0.29351				H	-3.99569	4.60398	-2.59702
C	1.84319	1.32537	-0.47977	C	-3.23831	0.67097	0.80576
N	1.67598	2.66256	-0.82952	C	-4.43836	1.33308	1.11148
C	2.89769	3.34253	-0.88418	C	-5.66935	0.77216	0.73715
C	3.86878	2.43657	-0.57733	C	-5.69670	-0.44955	0.04399
N	3.22649	1.21678	-0.33470	C	-4.49794	-1.11017	-0.26713
C	0.45257	3.29296	-1.28600	H	-2.27470	1.11464	1.07531
C	3.98845	-0.01430	-0.22377	H	-4.40808	2.29168	1.64031
H	4.94914	2.53387	-0.51047	H	-6.60522	1.28919	0.97515
H	2.95182	4.39685	-1.14185	H	-6.65273	-0.88654	-0.26416
C	1.02656	-1.22926	-1.59357	H	-4.52687	-2.04744	-0.83272
O	1.43805	-1.99396	-2.39817	C	-2.30805	-3.48075	-2.19408
P	-1.63854	-1.41617	-0.27429	C	-2.62962	-3.94082	-3.48358
C	-1.63319	-2.96431	0.77831	C	-2.72323	-3.03943	-4.55368
C	-3.25655	-0.56159	0.12480	C	-2.48956	-1.67118	-4.33168
				C	-2.16005	-1.21125	-3.04907

H	-2.24098	-4.19313	-1.36643
H	-2.80694	-5.00940	-3.64687
H	-2.97370	-3.39938	-5.55726
H	-2.55796	-0.96000	-5.16209
H	-1.96304	-0.14647	-2.88361
C	-2.76621	-3.47980	1.43860
C	-2.66846	-4.65541	2.20076
C	-1.44168	-5.32971	2.30903
C	-0.30722	-4.81944	1.65718
C	-0.40043	-3.64036	0.90202
H	-3.72470	-2.95634	1.37131
H	-3.55518	-5.04197	2.71491
H	-1.36834	-6.24522	2.90569
H	0.65623	-5.33309	1.74348
H	0.48979	-3.23241	0.41074

TS(5-6)_1,2,4-C6F3H3_1

SCF (BP86) Energy =	-2365.23916631		
Enthalpy 0K =	-2364.485018		
Enthalpy 298K =	-2364.430186		
Free Energy 298K =	-2364.579867		
SCRF (PCM,THF) Energy =	-2365.25488278		
Imaginary Frequency =	-185.7845 cm-1		
Ru	-0.18723	0.26812	0.30622
C	-1.50446	1.91659	0.15322
N	-1.10634	3.22344	-0.07419
C	-2.19600	4.09257	-0.13144
C	-3.31250	3.33824	0.07820
N	-2.88285	2.02265	0.25540
C	0.25231	3.71653	-0.18884
C	-3.82426	0.95512	0.52967
H	-4.36482	3.60406	0.12369
H	-2.06766	5.15585	-0.31306
C	-0.40180	0.14656	2.10053
O	-0.53177	0.06771	3.27521
P	1.58009	-1.34308	0.49540
C	2.51491	-1.28562	2.12070
C	1.02852	-3.12017	0.39318
C	3.02466	-1.20495	-0.68158
H	-0.01954	0.62511	-1.62466
H	0.92706	1.34521	0.58483
C	-0.58196	-0.27268	-2.06970
C	-1.48976	-1.08035	-1.32337
C	-1.77176	-2.41860	-1.69126
C	0.12841	-0.93657	-3.11303
C	-1.11374	-2.96862	-2.78175
C	-0.15523	-2.23368	-3.51127
H	-2.15464	-0.60689	-0.58143
F	-1.49435	1.15544	-2.85036
H	-2.50986	-3.00290	-1.13761
F	1.07696	-0.22536	-3.78426
F	-1.38149	-4.24749	-3.17420
H	0.36975	-2.67953	-4.35939
C	1.37035	-3.97618	-0.67193
C	0.83906	-5.27579	-0.73557
C	-0.03372	-5.73371	0.26198
C	-0.38663	-4.88238	1.32338
C	0.13154	-3.58100	1.38409
H	2.04242	-3.62756	-1.46088
H	1.10564	-5.92685	-1.57429
H	-0.44541	-6.74702	0.20980
H	-1.07282	-5.22900	2.10350
H	-0.16139	-2.91928	2.20668
C	4.08376	-2.13987	-0.64746
C	5.19645	-1.97928	-1.48492
C	5.27107	-0.87771	-2.35547
C	4.23167	0.06321	-2.38062
C	3.11325	-0.09755	-1.54545

H	4.04306	-2.98953	0.04183
H	6.00990	-2.71193	-1.45294
H	6.14184	-0.75290	-3.00782
H	4.28296	0.92561	-3.05280
H	2.31100	0.64522	-1.56132
C	2.91079	-2.44579	2.81600
C	3.66972	-2.34219	3.99386
C	4.04772	-1.08287	4.48362
C	3.66147	0.07681	3.79143
C	2.89681	-0.02230	2.61974
H	2.62064	-3.43337	2.44477
H	3.96494	-3.25181	4.52788
H	4.63835	-1.00437	5.40244
H	3.94936	1.06395	4.16838
H	2.58739	0.88435	2.08853
C	-4.06439	0.57754	1.87060
C	-4.96994	-0.47698	2.10309
C	-5.65222	-1.11724	1.05589
C	-5.44405	-0.65169	-0.25696
C	-4.54853	0.39167	-0.55423
C	-3.46668	1.31295	3.05129
H	-5.15468	-0.78999	3.13805
C	-6.59094	-2.27367	1.32716
H	-6.00206	-1.10751	-1.08360
C	-4.41122	0.90863	-1.96699
C	0.78331	3.98738	-1.47178
C	2.10342	4.47899	-1.53048
C	2.86853	4.72849	-0.37809
C	2.27176	4.50699	0.87769
C	0.96258	4.01037	1.00038
C	-0.02773	3.81044	-2.73322
H	2.53535	4.68749	-2.51680
C	4.29516	5.22481	-0.48152
H	2.83475	4.73682	1.79057
C	0.34193	3.81144	2.36468
H	0.60812	3.96900	-3.61919
H	-0.50935	2.81213	-2.80713
H	-0.84391	4.55595	-2.77967
H	-0.66473	4.26082	2.42377
H	0.23077	2.73972	2.60292
H	0.96700	4.27150	3.14641
H	4.54807	5.90700	0.34752
H	5.01173	4.38389	-0.44046
H	4.47044	5.75799	-1.43036
H	-4.98031	0.26905	-2.66050
H	-4.82678	1.93086	-2.04774
H	-3.35743	0.96097	-2.31171
H	-7.47220	-2.24314	0.66453
H	-6.08797	-3.24243	1.15185
H	-6.94531	-2.27191	2.37098
H	-2.65191	1.98986	2.76010
H	-4.24602	1.91882	3.54935
H	-3.06642	0.61051	3.79872

TS(2-3)_1,2,4-C6F3H3_2

SCF (BP86) Energy =	-2365.23405417		
Enthalpy 0K =	-2364.482831		
Enthalpy 298K =	-2364.427740		
Free Energy 298K =	-2364.577759		
SCRF (PCM,THF) Energy =	-2365.24703268		
Lowest frequency =	-598.9916 cm-1		
Ru	0.26166	-0.14872	-0.29408
C	1.90114	1.09350	-0.58498
N	1.87124	2.44614	-0.91202
C	3.15876	2.97583	-1.05132
C	4.03336	1.95567	-0.82305
N	3.26783	0.81807	-0.54258
C	0.70384	3.22813	-1.27087

C	3.88125	-0.49699	-0.49217
H	5.11956	1.92224	-0.83406
H	3.32072	4.02028	-1.30379
C	0.69457	-1.31886	-1.66576
O	0.94096	-2.10374	-2.51675
P	-1.85261	-1.22929	-0.12064
C	-1.93857	-2.78263	0.92043
C	-3.32366	-0.20163	0.41434
C	-2.49397	-1.84627	-1.77427
H	-0.08748	0.82668	1.21295
H	-0.47113	0.75120	-1.33553
C	0.44863	0.49804	2.57504
C	-0.65237	0.22346	3.44549
C	-0.96288	1.02081	4.53921
C	1.35086	1.50597	3.02602
C	-0.11701	2.08352	4.91557
C	1.02662	2.28774	4.13695
F	-1.46947	-0.81518	3.11411
F	1.07789	-0.69833	2.01714
H	-1.85972	0.77806	5.11655
H	2.25529	1.72155	2.45678
H	-0.32693	2.71575	5.77993
F	1.88453	3.29298	4.47458
C	4.36480	-1.01952	0.72863
C	4.97120	-2.29068	0.70387
C	5.12146	-3.02865	-0.48199
C	4.68939	-2.44199	-1.68547
C	4.08472	-1.17421	-1.72102
C	4.27833	-0.26083	2.03217
H	5.34519	-2.70733	1.64697
C	5.73356	-4.41291	-0.46868
H	4.83490	-2.97925	-2.63014
C	3.73507	-0.53794	-3.04783
H	2.72997	-0.09131	-3.04171
H	4.45055	0.26720	-3.29854
H	3.76942	-1.28375	-3.85649
H	5.04321	-0.62187	2.73840
H	4.43028	0.82181	1.88836
H	3.29083	-0.39540	2.50117
H	6.38159	-4.56116	0.41072
H	4.94926	-5.19127	-0.43407
H	6.33446	-4.59936	-1.37459
C	0.16843	4.14955	-0.34372
C	-0.92936	4.93048	-0.75140
C	-1.48829	4.82419	-2.03679
C	-0.89834	3.92433	-2.94305
C	0.20202	3.12282	-2.59058
C	0.74567	4.30906	1.04168
H	-1.35385	5.64714	-0.03796
C	-2.69461	5.64831	-2.43294
H	-1.29600	3.84909	-3.96249
C	0.82359	2.19088	-3.60513
H	1.82714	4.52999	1.01756
H	0.24516	5.12817	1.58146
H	0.62566	3.38619	1.63348
H	0.63455	1.13753	-3.33377
H	0.40471	2.37084	-4.60783
H	1.91829	2.32164	-3.66208
H	-2.74276	6.59382	-1.86784
H	-2.68425	5.89099	-3.50866
H	-3.63234	5.09845	-2.23164
C	-3.10916	1.00975	1.09962
C	-4.19685	1.79975	1.50565
C	-5.51017	1.38924	1.22864
C	-5.73333	0.18961	0.53230
C	-4.64729	-0.59867	0.12081
H	-2.08252	1.33585	1.29361
H	-4.01401	2.74046	2.03584

H	-6.35830	2.00630	1.54453
H	-6.75483	-0.13030	0.29970
H	-4.82913	-1.51737	-0.44673
C	-2.88827	-3.17995	-1.99608
C	-3.36030	-3.58136	-3.25861
C	-3.45072	-2.65521	-4.30763
C	-3.06257	-1.32143	-4.09212
C	-2.58337	-0.92075	-2.83716
H	-2.82503	-3.91070	-1.18427
H	-3.65761	-4.62363	-3.41743
H	-3.81856	-2.96951	-5.29017
H	-3.12754	-0.59154	-4.90641
H	-2.26745	0.11599	-2.67792
C	-3.06746	-3.17792	1.66516
C	-3.04309	-4.36753	2.41118
C	-1.89484	-5.17560	2.41912
C	-0.76436	-4.78574	1.68274
C	-0.78336	-3.59319	0.94331
H	-3.96342	-2.54998	1.67627
H	-3.92487	-4.66020	2.99155
H	-1.87845	-6.10182	3.00340
H	0.13927	-5.40456	1.69038
H	0.10615	-3.27981	0.38556

TS (5-6) _1,2,4-C6F3H3 _2

SCF (BP86) Energy =	-2365.24236192	
Enthalpy 0K =	-2364.488155	
Enthalpy 298K =	-2364.433333	
Free Energy 298K =	-2364.582491	
SCRF (PCM,THF) Energy =	-2365.25832108	
Imaginary Frequency =	-207.1062	cm-1
Ru	-0.18340	0.21246 0.28471
C	-1.48023	1.88508 0.25031
N	-1.06289	3.19858 0.11767
C	-2.13944	4.08512 0.13320
C	-3.26580	3.33374 0.29507
N	-2.85555	2.00258 0.37121
C	0.30164	3.67712 0.01129
C	-3.81371	0.93052 0.55788
H	-4.31381	3.61028 0.36728
H	-1.99591	5.15678 0.02881
C	-0.37025	0.00863 2.07282
O	-0.48938	-0.12297 3.24277
P	1.60913	-1.39059 0.34840
C	2.40213	-1.55733 2.03928
C	1.17771	-3.15518 -0.07612
C	3.13448	-1.01478 -0.66387
H	-0.11159	0.72802 -1.65257
H	0.94676	1.25373 0.61460
C	-0.60087	-0.19322 -2.10648
C	-1.52541	-1.01116 -1.40064
C	-1.80656	-2.30746 -1.87273
C	0.08297	-0.79145 -3.19744
C	-1.19688	-2.84857 -2.99957
C	-0.23289	-2.05806 -3.66780
H	-2.19176	-0.59061 -0.62936
F	-1.53326	1.38085 -2.80897
F	-2.73305	-3.04175 -1.19669
F	1.03601	-0.05247 -3.83659
H	-1.45839	-3.84999 -3.34613
H	0.29275	-2.43933 -4.54808
C	1.88687	-3.93153 -1.01331
C	1.48952	-5.25233 -1.28180
C	0.38700	-5.81002 -0.61679
C	-0.32984	-5.03855 0.31339
C	0.05644	-3.71625 0.57492
H	2.74685	-3.50658 -1.53871
H	2.04622	-5.84466 -2.01590

H	0.08097	-6.84016	-0.82768
H	-1.20028	-5.46015	0.82630
H	-0.52103	-3.11079	1.28222
C	4.33320	-1.73282	-0.44932
C	5.48334	-1.42917	-1.19178
C	5.45376	-0.39907	-2.14802
C	4.27143	0.32625	-2.35522
C	3.11678	0.02252	-1.61438
H	4.36996	-2.52114	0.30983
H	6.40610	-1.99281	-1.01744
H	6.35380	-0.16040	-2.72461
H	4.23961	1.13323	-3.09407
H	2.20305	0.59616	-1.78066
C	2.56442	-2.79148	2.69751
C	3.19229	-2.84632	3.95450
C	3.66905	-1.67437	4.55943
C	3.51418	-0.44060	3.90429
C	2.88149	-0.38051	2.65494
H	2.19997	-3.71265	2.23330
H	3.30834	-3.81217	4.45780
H	4.15756	-1.71964	5.53845
H	3.88114	0.47985	4.37069
H	2.75369	0.58486	2.15281
C	-4.05809	0.44368	1.86209
C	-4.97608	-0.61635	2.00497
C	-5.66496	-1.15724	0.90784
C	-5.45440	-0.58166	-0.36012
C	-4.54812	0.47303	-0.56931
C	-3.44997	1.06537	3.10146
H	-5.16405	-1.01464	3.00964
C	-6.61299	-2.32492	1.07778
H	-6.01678	-0.96031	-1.22183
C	-4.40550	1.10651	-1.93271
C	0.81082	4.03051	-1.26102
C	2.13933	4.49989	-1.31237
C	2.93263	4.65155	-0.16203
C	2.35639	4.35504	1.08770
C	1.03995	3.87586	1.20310
C	-0.03042	3.96499	-2.51305
H	2.55527	4.77069	-2.29040
C	4.36747	5.12436	-0.26151
H	2.94137	4.51110	2.00237
C	0.44088	3.60071	2.56394
H	0.59058	4.17766	-3.39835
H	-0.53957	2.98492	-2.65259
H	-0.82902	4.73038	-2.48430
H	-0.56050	4.05370	2.66718
H	0.32416	2.51830	2.74267
H	1.08349	4.00930	3.35999
H	4.65834	5.72511	0.61660
H	5.06391	4.26737	-0.31486
H	4.53078	5.73511	-1.16472
H	-4.99338	0.54135	-2.67382
H	-4.79888	2.14065	-1.92263
H	-3.35040	1.16766	-2.28043
H	-7.51782	-2.20481	0.45812
H	-6.13204	-3.27056	0.76773
H	-6.92825	-2.44253	2.12746
H	-2.68083	1.81360	2.86512
H	-4.23742	1.56640	3.69372
H	-2.98623	0.30346	3.74725

TS (2-3)_1,2,4-C6F3H3_4

SCF (BP86) Energy =	-2365.22940673
Enthalpy 0K =	-2364.478276
Enthalpy 298K =	-2364.423072
Free Energy 298K =	-2364.573942
SCRF (PCM,THF) Energy =	-2365.24276537

Lowest frequency = -591.2223 cm-1			
Ru	0.42898	-0.06482	-0.35717
C	1.91293	1.38100	-0.21801
N	1.76390	2.74609	-0.44357
C	2.96996	3.43520	-0.27635
C	3.91319	2.50717	0.05127
N	3.26871	1.26546	0.08344
C	0.59019	3.41542	-0.96854
C	4.03115	0.03401	0.17786
H	4.97516	2.60259	0.26149
H	3.03500	4.51126	-0.41335
C	1.29199	-1.07824	-1.64539
O	1.81580	-1.77801	-2.44382
P	-1.52741	-1.37645	-0.65845
C	-1.67496	-2.90812	0.41036
C	-3.17426	-0.51357	-0.43546
C	-1.74615	-2.07914	-2.38168
H	-0.35714	0.69793	1.12196
H	-0.17453	0.81793	-1.49789
C	-0.14188	0.23706	2.48917
C	-1.32492	-0.36009	3.02426
C	-1.92823	0.18460	4.15384
C	0.48083	1.27285	3.25330
C	-1.35770	1.26583	4.84768
C	-0.14774	1.79560	4.39121
H	-1.78150	-1.22614	2.54173
F	0.81732	-0.78007	1.95003
F	-3.07749	-0.36011	4.62547
H	1.42476	1.69633	2.90633
F	-1.97826	1.77016	5.94769
H	0.30809	2.62133	4.94611
C	4.31062	-0.54127	1.43779
C	5.08259	-1.71903	1.46365
C	5.58519	-2.31350	0.29403
C	5.33689	-1.67322	-0.93387
C	4.57888	-0.49319	-1.01824
C	3.83157	0.06939	2.73347
H	5.30174	-2.17671	2.43595
C	6.37207	-3.60531	0.35066
H	5.75141	-2.09663	-1.85643
C	4.41671	0.21337	-2.34572
H	3.37040	0.49374	-2.53917
H	5.01556	1.14243	-2.37566
H	4.75306	-0.43185	-3.17160
H	4.44502	-0.28557	3.57710
H	3.88272	1.17097	2.71181
H	2.78369	-0.20773	2.93050
H	6.83781	-3.75328	1.33883
H	5.71674	-4.47556	0.16251
H	7.16826	-3.62901	-0.41224
C	-0.24144	4.15329	-0.09750
C	-1.33835	4.83582	-0.65629
C	-1.61517	4.80719	-2.03423
C	-0.73888	4.09270	-2.87145
C	0.37412	3.39693	-2.36739
C	0.02631	4.22532	1.38667
H	-1.99098	5.41127	0.01135
C	-2.82600	5.51722	-2.60076
H	-0.91706	4.08300	-3.95365
C	1.30645	2.66323	-3.30383
H	1.05656	4.55822	1.60409
H	-0.66709	4.92927	1.87340
H	-0.09620	3.24001	1.86861
H	1.22827	1.57209	-3.15357
H	1.06131	2.88810	-4.35387
H	2.36092	2.94040	-3.13044
H	-3.11815	6.37942	-1.97877
H	-2.64079	5.87974	-3.62566

H	-3.69633	4.83718	-2.64760	F	0.57771	-3.41868	-3.86782
C	-3.23201	0.67483	0.31886	C	1.67493	-3.87510	-0.44971
C	-4.45699	1.33383	0.51247	C	1.26552	-5.21932	-0.41407
C	-5.63361	0.81713	-0.05188	C	0.45866	-5.68643	0.63343
C	-5.58257	-0.36034	-0.81666	C	0.04708	-4.80067	1.64412
C	-4.35993	-1.02205	-1.01060	C	0.44300	-3.45627	1.60549
H	-2.30630	1.08392	0.73680	H	2.29408	-3.52278	-1.27925
H	-4.48827	2.25530	1.10323	H	1.57407	-5.89739	-1.21613
H	-6.58805	1.33336	0.09728	H	0.14134	-6.73407	0.65789
H	-6.49516	-0.76304	-1.26923	H	-0.59067	-5.15426	2.46127
H	-4.32483	-1.92927	-1.62290	H	0.10347	-2.76873	2.38819
C	-2.08959	-3.42413	-2.62244	C	4.18599	-1.78928	-0.66777
C	-2.25823	-3.88877	-3.93869	C	5.24003	-1.57576	-1.56862
C	-2.09345	-3.01503	-5.02362	C	5.17951	-0.51413	-2.48712
C	-1.75338	-1.67162	-4.78969	C	4.06438	0.33777	-2.49517
C	-1.57543	-1.20740	-3.47873	C	3.00495	0.12185	-1.59823
H	-2.22226	-4.11339	-1.78293	H	4.25238	-2.60619	0.05815
H	-2.51912	-4.93841	-4.11196	H	6.11315	-2.23650	-1.54786
H	-2.22419	-3.37901	-6.04821	H	6.00411	-0.34772	-3.18824
H	-1.61679	-0.98439	-5.63160	H	4.01386	1.17528	-3.19858
H	-1.29002	-0.16551	-3.29816	H	2.14539	0.80018	-1.59515
C	-2.87551	-3.34485	1.00793	C	3.16345	-2.03327	2.88135
C	-2.88770	-4.49534	1.81533	C	3.95491	-1.80865	4.02042
C	-1.70666	-5.22361	2.02699	C	4.26229	-0.49993	4.42187
C	-0.50677	-4.79442	1.43497	C	3.77308	0.58776	3.67966
C	-0.48811	-3.63933	0.63965	C	2.97603	0.36774	2.54679
H	-3.80130	-2.78254	0.85098	H	2.92965	-3.05853	2.57922
H	-3.82457	-4.81903	2.28125	H	4.33094	-2.66295	4.59355
H	-1.71871	-6.11815	2.65859	H	4.87805	-0.32717	5.31079
H	0.42071	-5.35195	1.60302	H	4.00544	1.61274	3.98754
H	0.45327	-3.29102	0.20048	H	2.58805	1.21857	1.97636
TS (5-6)_1,2,4-C6F3H3_4				C	-4.19481	0.64053	1.83814
SCF (BP86) Energy =				C	-5.12736	-0.38379	2.09516
Enthalpy 0K =				C	-5.78320	-1.07218	1.06077
Enthalpy 298K =				C	-5.52598	-0.68057	-0.26677
Free Energy 298K =				C	-4.60842	0.33677	-0.58895
SCRF (PCM,THF) Energy =				C	-3.58632	1.40349	2.99499
Imaginary Frequency =				H	-5.35760	-0.63228	3.13842
-208.5478 cm-1				C	-6.75129	-2.19604	1.36370
Ru	-0.19790	0.31091	0.33572	H	-6.06711	-1.16915	-1.08583
C	-1.58029	1.90290	0.07293	C	-4.42121	0.77878	-2.02111
N	-1.20561	3.19828	-0.24866	C	0.61999	3.85590	-1.77437
C	-2.30630	4.04887	-0.34531	C	1.92573	4.36635	-1.92597
C	-3.40926	3.29558	-0.07315	C	2.72218	4.74218	-0.83020
N	-2.96000	1.99859	0.18245	C	2.17255	4.63196	0.46136
C	0.13929	3.69961	-0.45252	C	0.87993	4.12356	0.67714
C	-3.90722	0.94305	0.48721	C	-0.22923	3.54101	-2.98233
H	-4.46512	3.54831	-0.03372	H	2.31870	4.49124	-2.94238
H	-2.19395	5.09966	-0.59695	C	4.13179	5.25694	-1.03098
C	-0.32552	0.37308	2.14157	H	2.75946	4.96167	1.32734
O	-0.40352	0.41181	3.32388	C	0.30706	4.04658	2.07410
P	1.67081	-1.16215	0.55983	H	0.35622	3.68564	-3.90495
C	2.66372	-0.94595	2.13702	H	-0.64487	2.50780	-2.97541
C	1.27647	-2.98365	0.56589	H	-1.09833	4.22304	-3.03705
C	3.05003	-0.95086	-0.68610	H	-0.70310	4.48876	2.12504
H	-0.15492	0.45881	-1.61587	H	0.21628	3.00121	2.41507
H	0.87094	1.45960	0.45197	H	0.95103	4.58404	2.78814
C	-0.60602	-0.55346	-1.90460	H	4.39379	6.02334	-0.28226
C	-1.58222	-1.21341	-1.10092	H	4.87031	4.44022	-0.93195
C	-1.84767	-2.59120	-1.28194	H	4.26291	5.69742	-2.03304
C	0.18692	-1.33720	-2.79292	H	-5.02340	0.14538	-2.69211
C	-1.14023	-3.31539	-2.23004	H	-4.76702	1.82092	-2.15501
C	-0.13189	-2.67367	-2.98484	H	-3.36144	0.74748	-2.35798
H	-2.29321	-0.63639	-0.49820	H	-7.58383	-2.21902	0.64080
F	-1.51658	0.81225	-2.93513	H	-6.24775	-3.17884	1.30941
H	-2.63320	-3.08519	-0.70393	H	-7.17704	-2.10244	2.37631
H	1.00305	-0.89468	-3.36615	H	-3.27198	2.41707	2.70040
F	-1.38556	-4.63373	-2.44794	H	-4.32034	1.49644	3.81259

H -2.69920 0.89408 3.40457

TS(2-3)_1,2-C6F2H4

SCF (BP86) Energy = -2266.00010495
Enthalpy 0K = -2265.240852
Enthalpy 298K = -2265.186720
Free Energy 298K = -2265.334417
SCRF (PCM,THF) Energy = -2266.01304369
Lowest frequency = -598.9395 cm-1

Ru 0.31530 -0.02778 -0.19345
C 1.85033 1.36892 -0.22014
N 1.71283 2.74792 -0.35296
C 2.95252 3.39674 -0.35082
C 3.90500 2.42971 -0.22589
N 3.23377 1.20382 -0.14869
C 0.49425 3.47199 -0.65844
C 3.96035 -0.04852 -0.25886
H 4.98956 2.48791 -0.18754
H 3.03053 4.47653 -0.44494
C 0.91420 -0.96439 -1.67616
O 1.27174 -1.60773 -2.60347
P -1.70828 -1.27933 -0.29782
C -1.71471 -2.97457 0.49684
C -3.28332 -0.45808 0.29520
C -2.21897 -1.68729 -2.05891
H -0.17211 0.69386 1.42359
H -0.43955 0.94417 -1.15308
C 0.31911 0.20298 2.73414
C -0.78055 -0.30039 3.49406
C -1.19154 0.26271 4.69613
C 1.11656 1.18467 3.39616
C -0.43722 1.29788 5.28223
C 0.71995 1.74026 4.62078
F -1.49825 -1.32622 2.95468
F 1.07465 -0.84715 2.02264
H -2.08248 -0.14999 5.17941
H 2.01551 1.54322 2.89032
H -0.74077 1.72816 6.24034
H 1.34237 2.52366 5.06699
C 4.43851 -0.70858 0.89559
C 5.16043 -1.90472 0.71588
C 5.42795 -2.43732 -0.55616
C 4.99276 -1.71348 -1.68122
C 4.27466 -0.51183 -1.56139
C 4.22595 -0.16910 2.29036
H 5.53127 -2.42734 1.60596
C 6.16515 -3.74976 -0.71449
H 5.22531 -2.08650 -2.68571
C 3.91584 0.28384 -2.79648
H 2.86487 0.60855 -2.78808
H 4.53967 1.19347 -2.87525
H 4.07763 -0.31654 -3.70466
H 4.98012 -0.58024 2.98059
H 4.29823 0.93091 2.32023
H 3.22899 -0.44341 2.67004
H 6.78664 -3.97459 0.16784
H 5.45594 -4.58854 -0.83947
H 6.81838 -3.74339 -1.60321
C -0.16577 4.19268 0.36138
C -1.31505 4.92604 0.01135
C -1.80689 4.96496 -1.30488
C -1.09539 4.26794 -2.29823
C 0.06076 3.52293 -2.00531
C 0.33444 4.19418 1.78547
H -1.83577 5.48715 0.79675
C -3.06949 5.72839 -1.64302
H -1.44066 4.31192 -3.33839
C 0.80892 2.81056 -3.10846

H 1.39549 4.49348 1.84953
H -0.25255 4.89213 2.40320
H 0.26136 3.19249 2.24202
H 0.69808 1.71640 -3.00980
H 0.42472 3.10990 -4.09643
H 1.88974 3.03275 -3.07835
H -3.22642 6.57674 -0.95642
H -3.04256 6.12052 -2.67337
H -3.95848 5.07582 -1.56530
C -3.20304 0.64363 1.16867
C -4.37073 1.27762 1.62306
C -5.63069 0.81995 1.20688
C -5.71997 -0.26904 0.32379
C -4.55376 -0.90105 -0.13534
H -2.21784 1.01023 1.47324
H -4.29217 2.13402 2.30122
H -6.54120 1.31557 1.56080
H -6.69904 -0.62325 -0.01665
H -4.63091 -1.73108 -0.84547
C -2.49659 -2.99778 -2.49381
C -2.87491 -3.24006 -3.82651
C -2.98762 -2.17744 -4.73451
C -2.71596 -0.86635 -4.30634
C -2.32990 -0.62329 -2.98079
H -2.41502 -3.83456 -1.79371
H -3.08147 -4.26573 -4.15108
H -3.28237 -2.36782 -5.77201
H -2.79906 -0.03023 -5.00924
H -2.10364 0.39795 -2.65544
C -2.84203 -3.56296 1.10367
C -2.75442 -4.84650 1.66695
C -1.54361 -5.55638 1.62763
C -0.41475 -4.97428 1.02841
C -0.49761 -3.68850 0.47243
H -3.78748 -3.01417 1.15119
H -3.63620 -5.29005 2.14214
H -1.47799 -6.55635 2.06960
H 0.53670 -5.51612 1.00173
H 0.38879 -3.22665 0.02383

TS(5-6)_1,2-C6F2H4

SCF (BP86) Energy = -2266.00716848
Enthalpy 0K = -2265.244989
Enthalpy 298K = -2265.191102
Free Energy 298K = -2265.338425
SCRF (PCM,THF) Energy = -2266.02266669
Imaginary Frequency = -187.5037 cm-1

Ru -0.24737 0.13068 0.24752
C -1.72668 1.63969 0.22570
N -1.46885 2.99682 0.13296
C -2.64564 3.74596 0.13252
C -3.67635 2.86034 0.24535
N -3.10914 1.58718 0.30829
C -0.17022 3.64063 0.09500
C -3.93162 0.40397 0.46589
H -4.75172 3.00684 0.29170
H -2.63104 4.82928 0.05410
C -0.47583 -0.18314 2.01629
O -0.61838 -0.38477 3.17433
P 1.69291 -1.28604 0.32304
C 2.51731 -1.34701 2.00724
C 1.39847 -3.08922 -0.05285
C 3.17498 -0.81355 -0.71279
H -0.10543 0.71132 -1.63975
H 0.74601 1.27923 0.66083
C -0.54062 -0.20187 -2.17943
C -1.35780 -1.17870 -1.54140
C -1.48751 -2.48300 -2.07074

C	0.23052	-0.65553	-3.28528
C	-0.78723	-2.85532	-3.21924
C	0.08389	-1.92151	-3.83063
H	-2.06316	-0.86635	-0.74915
F	-1.63091	1.22234	-2.80113
H	-2.16641	-3.18659	-1.57984
F	1.09538	0.23277	-3.85941
H	-0.90431	-3.85368	-3.64964
H	0.66551	-2.17900	-4.72122
C	2.06129	-3.79346	-1.07605
C	1.75707	-5.14428	-1.31772
C	0.79327	-5.80404	-0.54126
C	0.11893	-5.10401	0.47415
C	0.41049	-3.75301	0.70936
H	2.81214	-3.28935	-1.69074
H	2.27837	-5.67938	-2.11864
H	0.56180	-6.85778	-0.72939
H	-0.64154	-5.60810	1.08010
H	-0.13241	-3.20787	1.48944
C	4.39732	-1.51096	-0.57970
C	5.51900	-1.12270	-1.32573
C	5.43730	-0.02762	-2.20376
C	4.23195	0.67813	-2.32799
C	3.10556	0.28965	-1.58302
H	4.47536	-2.35056	0.11893
H	6.46048	-1.67138	-1.21547
H	6.31504	0.27622	-2.78406
H	4.15945	1.53426	-3.00614
H	2.17331	0.84993	-1.68124
C	2.89971	-2.54848	2.63538
C	3.55689	-2.52080	3.87777
C	3.84510	-1.29669	4.49891
C	3.47107	-0.09489	3.87415
C	2.80799	-0.11860	2.63901
H	2.68146	-3.50943	2.16000
H	3.84365	-3.46268	4.35775
H	4.35647	-1.27751	5.46708
H	3.68945	0.86537	4.35341
H	2.50719	0.82007	2.16090
C	-4.14750	-0.11454	1.76333
C	-4.93339	-1.27823	1.88282
C	-5.52556	-1.89418	0.76833
C	-5.35316	-1.29364	-0.49374
C	-4.57543	-0.13596	-0.67901
C	-3.65304	0.57498	3.01734
H	-5.09699	-1.69939	2.88241
C	-6.33364	-3.16595	0.91672
H	-5.84696	-1.73178	-1.36938
C	-4.48152	0.51898	-2.03655
C	0.33850	4.09829	-1.14344
C	1.59823	4.73113	-1.12618
C	2.32284	4.94005	0.05990
C	1.74323	4.52826	1.27492
C	0.49422	3.88509	1.32132
C	-0.43879	3.96876	-2.43139
H	2.01315	5.08490	-2.07780
C	3.68882	5.59254	0.03419
H	2.27032	4.72205	2.21717
C	-0.11335	3.48546	2.64701
H	0.18825	4.27154	-3.28558
H	-0.82360	2.94080	-2.60803
H	-1.32110	4.63649	-2.42203
H	-1.16586	3.80896	2.72647
H	-0.10185	2.39032	2.78124
H	0.44598	3.93691	3.48184
H	3.86794	6.19414	0.94116
H	4.49032	4.83264	-0.01575
H	3.80686	6.25011	-0.84280

H	-4.95557	-0.12029	-2.79855
H	-5.02167	1.48480	-2.03703
H	-3.43663	0.73412	-2.34633
H	-7.19787	-3.17818	0.23144
H	-5.72110	-4.05558	0.68067
H	-6.70911	-3.29003	1.94575
H	-2.92052	1.36572	2.80502
H	-4.50366	1.03850	3.55034
H	-3.18099	-0.14114	3.70771

Model 3
1'

SCF (BP86) Energy =	-767.141462647		
Enthalpy 0K =	-766.769517		
Enthalpy 298K =	-766.741726		
Free Energy 298K =	-766.827654		
Ru	-0.16211	-0.38118	0.06484
C	1.89615	-0.54467	-0.07436
N	2.61776	-1.29095	-0.99381
C	3.98653	-1.25527	-0.73783
C	4.16227	-0.46807	0.36313
N	2.89370	-0.03958	0.75041
C	2.03257	-2.08715	-2.06960
C	2.66517	0.77135	1.94170
H	3.57939	1.34393	2.16384
H	1.82883	1.45920	1.75761
H	2.40553	0.14186	2.80816
H	5.06307	-0.17691	0.89697
H	4.70622	-1.78158	-1.35919
H	2.84867	-2.58692	-2.61415
H	1.45382	-1.44308	-2.74800
H	1.33994	-2.83068	-1.64626
C	-0.25724	-0.36482	1.95625
O	-0.39165	-0.39632	3.13500
P	-2.45040	-0.88216	-0.07487
C	-3.16488	-1.18790	-1.77563
C	-2.93802	-2.46436	0.79546
C	-3.74047	0.27677	0.64987
H	-0.17347	-0.54713	-1.60662
H	-0.07499	-2.01663	0.00634
P	-0.25874	1.92782	-0.49067
C	-1.43080	2.42607	-1.87041
C	-0.72565	3.21790	0.79631
C	1.31189	2.69936	-1.17410
H	1.16490	3.75680	-1.45328
H	2.11565	2.62768	-0.42477
H	1.62006	2.12224	-2.06013
H	-0.73925	4.23972	0.37899
H	-1.72149	2.97289	1.19854
H	-0.00732	3.17506	1.63089
H	-1.34678	3.49953	-2.11287
H	-1.19003	1.82268	-2.75948
H	-2.46849	2.20585	-1.57329
H	-4.01888	-2.66822	0.70622
H	-2.36021	-3.29231	0.35721
H	-2.66162	-2.38037	1.85814
H	-4.76077	-0.13319	0.55506
H	-3.50817	0.43515	1.71519
H	-3.69622	1.25141	0.13798
H	-4.22477	-1.49151	-1.72838
H	-3.06693	-0.27167	-2.37799
H	-2.56870	-1.97795	-2.25749

2'

SCF (BP86) Energy =	-640.780766357
Enthalpy 0K =	-640.521116
Enthalpy 298K =	-640.501043
Free Energy 298K =	-640.570934

Ru	-0.22807	-0.03903	0.02849
C	1.82134	0.15906	0.08352
N	2.59408	1.24736	-0.27949
C	3.94962	1.01698	-0.06470
C	4.05955	-0.24128	0.45817
N	2.76587	-0.75114	0.53569
C	2.05514	2.47922	-0.84895
C	2.44022	-2.05981	1.09208
H	4.93010	-0.80650	0.78097
H	4.70943	1.75639	-0.30442
C	-0.30253	-1.60555	-1.02547
O	-0.39230	-2.52948	-1.76194
P	-2.53463	0.27208	0.22099
C	-3.71911	-0.88392	-0.65620
C	-3.21168	0.20924	1.96979
C	-3.18102	1.93236	-0.34644
H	-0.25532	1.46611	0.81203
H	-0.28750	0.77089	-1.29948
H	3.19436	-2.79737	0.77445
H	2.40684	-2.02734	2.19499
H	1.45287	-2.35698	0.70695
H	2.75586	3.30421	-0.64641
H	1.90908	2.37788	-1.93737
H	1.08053	2.67200	-0.37503
H	-4.77293	-0.60633	-0.48420
H	-3.50353	-0.85772	-1.73602
H	-3.54628	-1.91169	-0.29983
H	-4.29522	0.41683	1.99495
H	-3.02527	-0.78985	2.39597
H	-2.67748	0.95469	2.57932
H	-4.26885	2.02482	-0.18695
H	-2.64882	2.71854	0.21017
H	-2.95369	2.05221	-1.41738

4'

SCF (BP86) Energy =	-1369.17362910	
Enthalpy 0K =	-1368.853360	
Enthalpy 298K =	-1368.823453	
Free Energy 298K =	-1368.913409	
Ru	-0.53578	0.57935 -0.22740
C	-2.49946	-0.10014 -0.07761
N	-3.29344	-0.60246 -1.09266
C	-4.58608	-0.87470 -0.65581
C	-4.63437	-0.54421 0.66699
N	-3.36404	-0.08295 1.00688
C	-2.86603	-0.84654 -2.47179
C	-3.06592	0.43967 2.33969
H	-2.02755	0.21158 2.60857
H	-3.20376	1.53248 2.37615
H	-3.74455	-0.03711 3.06347
H	-5.44498	-0.59800 1.38865
H	-5.34541	-1.28621 -1.31517
H	-3.71992	-1.26905 -3.02312
H	-2.02598	-1.55384 -2.48177
H	-2.54622	0.09425 -2.94261
C	-0.60101	1.86668 1.19104
O	-0.59023	2.79087 1.92403
P	1.45163	1.64064 -1.00562
C	1.07596	3.35062 -1.66221
C	2.86390	2.05432 0.15582
C	2.36272	0.91770 -2.46849
H	-0.53543	0.04361 -1.77989
H	-1.24127	1.72156 -1.10500
C	0.16671	-1.58307 -0.11408
C	0.11917	-1.12533 1.25186
C	1.35104	-0.92805 1.95214
C	1.45330	-1.89243 -0.68977
C	2.56936	-1.19452 1.36475

C	2.61299	-1.67898	0.02023
H	-0.75998	-1.37808	1.85005
F	-0.84064	-2.44478	-0.53499
F	1.30183	-0.48467	3.23142
F	1.50838	-2.32968	-1.96814
F	3.74128	-0.92794	1.98866
F	3.82287	-1.82144	-0.57126
H	3.16889	1.59574	-2.79521
H	2.79426	-0.05976	-2.21152
H	1.64181	0.77586	-3.28821
H	1.98943	3.85238	-2.02390
H	0.34854	3.26055	-2.48342
H	0.61823	3.94896	-0.85922
H	3.62682	2.66282	-0.35857
H	2.45891	2.62276	1.00815
H	3.33522	1.13969	0.54286

TS (4'-5')

SCF (BP86) Energy =	-1369.16172672	
Enthalpy 0K =	-1368.842979	
Enthalpy 298K =	-1368.813405	
Free Energy 298K =	-1368.902882	
Imaginary Frequency =	-553.1219	cm-1
Ru	-0.54899	0.62055 -0.15211
C	-2.47962	-0.14884 -0.09554
N	-3.26171	-0.52565 -1.16928
C	-4.52171	-0.95617 -0.76499
C	-4.55701	-0.85013 0.59598
N	-3.31060	-0.36744 0.98972
C	-2.82306	-0.52666 -2.56547
C	-2.99027	-0.06098 2.38444
H	-1.90532	-0.13602 2.53087
H	-3.31062	0.96049 2.64650
H	-3.50480	-0.78413 3.03621
H	-5.34691	-1.06857 1.30964
H	-5.26980	-1.30366 -1.47245
H	-3.70198	-0.69059 -3.20691
H	-2.08504	-1.32691 -2.72819
H	-2.35588	0.44018 -2.80052
C	-0.90225	1.92072 1.13806
O	-1.11239	2.78755 1.91576
P	1.41901	1.84339 -0.69095
C	1.04637	3.64557 -1.01470
C	2.83677	2.02499 0.52209
C	2.30617	1.39329 -2.27340
H	-0.18782	-0.44366 -1.44814
H	-1.15500	1.57825 -1.30468
C	0.28042	-1.53595 -0.49713
C	0.10636	-1.31166 0.93706
C	1.25810	-1.20186 1.77847
C	1.64556	-1.76862 -0.94619
C	2.53848	-1.36379 1.29848
C	2.71551	-1.64823 -0.09241
H	-0.79487	-1.72839 1.39560
F	-0.63491	-2.45224 -1.05724
F	1.05660	-0.95820 3.09650
F	1.84999	-1.97176 -2.27448
F	3.64146	-1.15124 2.05932
F	3.97724	-1.71941 -0.56959
H	3.61101	2.70096 0.12129
H	2.43665	2.44520 1.45877
H	3.29000	1.04985 0.74997
H	3.16439	2.06450 -2.44392
H	2.65592	0.35179 -2.24011
H	1.59232	1.49200 -3.10628
H	1.96066	4.20101 -1.28295
H	0.31346	3.71062 -1.83318
H	0.59694	4.08876 -0.11270

5'

SCF (BP86) Energy = -1369.16400420
Enthalpy 0K = -1368.842699
Enthalpy 298K = -1368.812844
Free Energy 298K = -1368.903060
Ru -0.59046 0.66702 -0.15546
C -2.48311 -0.19090 -0.10312
N -3.23814 -0.62544 -1.17353
C -4.46728 -1.13310 -0.76426
C -4.50867 -1.01520 0.59614
N -3.29532 -0.45213 0.98479
C -2.78398 -0.63082 -2.56467
C -2.97550 -0.13409 2.37790
H -3.48586 -0.85711 3.03259
H -1.88931 -0.20517 2.52295
H -3.30081 0.88680 2.63430
H -5.28397 -1.27429 1.31220
H -5.19117 -1.53590 -1.46756
H -3.65818 -0.75501 -3.22123
H -2.07271 -1.45636 -2.72637
H -2.28181 0.32435 -2.77738
C -1.03939 1.95118 1.06208
O -1.32965 2.80797 1.82950
P 1.36572 1.93553 -0.62762
C 0.98720 3.74879 -0.86382
C 2.79120 2.05123 0.58152
C 2.23126 1.55256 -2.24011
H -0.04943 -0.60999 -1.37531
H -1.16857 1.56355 -1.38462
C 0.36434 -1.49844 -0.61563
C 0.13412 -1.24998 0.83483
C 1.25345 -1.22099 1.73459
C 1.77086 -1.70886 -0.98545
C 2.55053 -1.39572 1.32175
C 2.79052 -1.63954 -0.07288
H -0.75789 -1.73799 1.24323
F -0.47552 -2.53855 -1.14371
F 0.98279 -1.02255 3.04915
F 2.04589 -1.86107 -2.31250
F 3.62185 -1.24427 2.14212
F 4.07422 -1.72675 -0.48156
H 3.56601 2.74307 0.21021
H 2.39994 2.42367 1.54177
H 3.23811 1.06174 0.75399
H 3.10917 2.20618 -2.37478
H 2.54818 0.50025 -2.27283
H 1.51759 1.72627 -3.06099
H 1.89734 4.31636 -1.11982
H 0.24252 3.84763 -1.66816
H 0.55014 4.15156 0.06286

TS (5'-6')

SCF (BP86) Energy = -1369.14447298
Enthalpy 0K = -1368.823649
Enthalpy 298K = -1368.793844
Free Energy 298K = -1368.884039
Imaginary Frequency = -385.8780 cm-1
Ru 0.62068 0.73458 -0.14349
C 2.42054 -0.27799 0.19364
N 3.11073 -0.36426 1.38024
C 4.29323 -1.07786 1.22811
C 4.36923 -1.45049 -0.08513
N 3.22010 -0.96284 -0.70143
C 2.61689 0.12683 2.67540
C 2.93320 -1.14548 -2.12521
H 3.41236 -2.07543 -2.46677
H 1.84623 -1.22380 -2.26734

H 3.31093 -0.29794 -2.71875
H 5.12559 -2.01124 -0.62754
H 4.96218 -1.26882 2.06273
H 3.42363 0.01486 3.41482
H 1.72214 -0.46806 2.95979
H 2.35313 1.19213 2.58068
C 1.26742 1.49402 -1.66503
O 1.68398 1.97462 -2.66345
P -1.17722 2.32011 -0.17355
H 0.09095 -0.20003 1.53931
H 1.32336 1.92655 0.63223
C -0.62844 -0.86376 0.94186
C -0.21973 -1.67098 -0.16770
C -1.19389 -2.34148 -0.94518
C -2.02080 -0.75343 1.19415
C -2.55251 -2.22292 -0.68216
C -2.95479 -1.42692 0.41945
H 0.80271 -2.04130 -0.23310
F 0.13445 -1.51214 2.65511
F -0.78401 -3.14897 -1.95321
F -2.47060 0.06244 2.18286
F -3.48659 -2.84695 -1.43142
F -4.27376 -1.24517 0.64601
C -2.89964 1.92830 -0.79375
C -1.52327 3.06907 1.50108
C -0.79145 3.84838 -1.17402
H -2.82977 1.50964 -1.81009
H -3.38217 1.18811 -0.13994
H -3.51529 2.84321 -0.81785
H -0.59472 3.52397 1.87940
H -2.31129 3.83758 1.43159
H -1.83839 2.27371 2.19076
H -0.68776 3.58247 -2.23707
H -1.58955 4.60010 -1.05980
H 0.16503 4.26922 -0.82739

6'

SCF (BP86) Energy = -1369.20796405
Enthalpy 0K = -1368.887434
Enthalpy 298K = -1368.856069
Free Energy 298K = -1368.951973
Ru -1.15842 -0.10019 0.03874
C -0.99111 1.96272 0.23242
N -0.61721 2.73089 1.31316
C -0.63354 4.08994 1.00508
C -1.02705 4.19432 -0.29893
N -1.23841 2.89522 -0.75359
C -0.19952 2.22596 2.62180
C -1.70038 2.56087 -2.10208
H -1.56882 3.44155 -2.74815
H -1.09968 1.73077 -2.49980
H -2.76354 2.27260 -2.09056
H -1.17265 5.06400 -0.93428
H -0.36135 4.85113 1.73136
H 0.88216 2.38182 2.76272
H -0.41494 1.15312 2.68090
H -0.75484 2.75343 3.41414
C -2.97463 -0.04229 -0.43489
O -4.10744 -0.02173 -0.77136
P -1.19016 -2.48133 -0.09646
C -2.52749 -3.32223 0.89536
C -1.48701 -3.14914 -1.81787
C 0.32801 -3.41796 0.43901
H -0.72315 -0.96589 2.14722
H -1.73893 -0.08594 1.48886
C 0.98498 -0.15956 0.21510
C 1.95563 -0.27151 1.23897
C 3.32405 -0.23983 0.93957

C	1.49126	-0.03764	-1.07765
C	3.78559	-0.10417	-0.38082
C	2.84589	-0.00396	-1.42056
H	1.65557	-0.42683	2.27918
F	-0.41847	-1.34458	2.99317
F	4.25179	-0.34897	1.92482
F	0.55357	0.04566	-2.11602
F	5.10797	-0.07643	-0.65781
F	3.26168	0.11641	-2.70209
H	-2.51465	-4.41456	0.74582
H	-2.35872	-3.09316	1.95901
H	-3.50748	-2.91789	0.59803
H	-1.49241	-4.25195	-1.82680
H	-2.45452	-2.77376	-2.18669
H	-0.69221	-2.78145	-2.48575
H	0.17574	-4.50579	0.34531
H	1.18406	-3.10298	-0.17642
H	0.53510	-3.15065	1.48629

TS(6'-3')

SCF (BP86) Energy =	-1369.19657756		
Enthalpy 0K =	-1368.876360		
Enthalpy 298K =	-1368.846049		
Free Energy 298K =	-1368.938281		
Imaginary Frequency =	-117.2321	cm-1	
Ru	1.16954	0.28570	0.07246
C	0.33370	2.16930	0.18040
N	0.35212	3.14581	-0.79197
C	-0.27783	4.31078	-0.35785
C	-0.71344	4.07018	0.91568
N	-0.34115	2.76352	1.22356
C	1.00774	2.99666	-2.09394
C	-0.62116	2.10233	2.49773
H	-1.54786	2.51623	2.92359
H	-0.74790	1.02640	2.30958
H	0.20907	2.24627	3.20790
H	-1.25854	4.69966	1.61404
H	-0.37157	5.18994	-0.98986
H	2.09267	3.16945	-1.99954
H	0.57920	3.73182	-2.79208
H	0.83893	1.97938	-2.47665
C	2.14410	0.53141	1.56604
O	2.71719	0.65749	2.60075
P	2.31741	-1.77226	-0.35688
C	3.93908	-1.47726	-1.23580
C	2.86036	-2.79009	1.11087
C	1.53784	-3.05957	-1.46399
H	-0.04252	-0.44206	-1.86715
H	2.42988	0.97937	-0.58756
C	-0.93692	-0.45849	-0.32119
C	-2.00059	0.32475	-0.86506
C	-3.34230	-0.03562	-0.73971
C	-1.35605	-1.60726	0.36851
C	-3.70880	-1.19205	-0.03019
C	-2.69978	-1.98273	0.53512
H	-1.78456	1.24368	-1.42008
F	0.46337	-0.23179	-2.69031
F	-4.32838	0.72298	-1.28033
F	-0.45162	-2.45292	0.96506
F	-5.00334	-1.53628	0.11460
F	-3.03635	-3.09103	1.23117
H	2.24751	-3.87500	-1.68139
H	0.64856	-3.46335	-0.95895
H	1.22817	-2.56978	-2.39921
H	4.47637	-2.42157	-1.42689
H	3.73036	-0.97103	-2.19106
H	4.56338	-0.81264	-0.61869
H	3.46496	-3.65541	0.79238

H	3.45232	-2.15586	1.78890
H	1.96738	-3.14032	1.64914

TS(2'-3')

SCF (BP86) Energy =	-1369.14226459	
Enthalpy 0K =	-1368.824947	
Enthalpy 298K =	-1368.794495	
Free Energy 298K =	-1368.888262	
Imaginary Frequency =	-571.0803	cm-1
Ru	-1.44385	0.03153 0.12075
C	-0.91528	2.02523 0.22981
N	-0.31605	2.69328 1.27865
C	-0.13570	4.04472 0.99464
C	-0.62034	4.24848 -0.26782
N	-1.08406	3.01500 -0.71943
C	0.05793	2.06772 2.54604
C	-1.69254	2.79378 -2.03199
H	-0.66399	5.14651 -0.87852
H	0.32688	4.73042 1.69956
C	-3.18866	0.38536 -0.38284
O	-4.30539	0.60995 -0.71174
P	-1.91980	-2.27582 0.33710
C	-3.64425	-2.66126 0.94454
C	-1.81740	-3.35170 -1.18985
C	-0.88679	-3.23257 1.56430
H	0.31787	-0.29639 0.44366
H	-1.94776	0.14032 1.60011
C	1.35967	-0.24143 -0.62258
C	2.07312	-1.47500 -0.57217
C	3.41077	-1.53104 -0.17685
C	2.15364	0.94315 -0.53880
C	4.15618	-0.35405 0.00905
C	3.49607	0.87126 -0.17343
F	1.38863	-2.64660 -0.71804
F	0.31734	-0.20082 -1.64684
F	4.00713	-2.73176 -0.01770
H	1.68904	1.92105 -0.67206
F	5.46070	-0.41275 0.36110
F	4.21023	2.01406 -0.02129
H	-2.79048	2.75337 -1.95364
H	-1.40194	3.61719 -2.70154
H	-1.32691	1.84357 -2.44682
H	0.93121	2.59121 2.96430
H	-0.77823	2.11032 3.26383
H	0.30556	1.01419 2.35211
H	-2.07067	-4.40112 -0.96292
H	-2.51716	-2.96113 -1.94575
H	-0.79477	-3.29437 -1.58994
H	-1.24540	-4.27090 1.66593
H	0.15652	-3.23155 1.21856
H	-0.94061	-2.72702 2.54124
H	-3.80152	-3.74800 1.04650
H	-3.79343	-2.17372 1.92068
H	-4.37879	-2.24645 0.23710

3'

SCF (BP86) Energy =	-740.075823760		
Enthalpy 0K =	-739.819945		
Enthalpy 298K =	-739.799040		
Free Energy 298K =	-739.870570		
Ru	-0.22785	0.01201	0.00856
C	1.85427	-0.10136	0.07871
N	2.75282	0.87287	0.47301
C	4.06895	0.44019	0.34940
C	4.01749	-0.83964	-0.12906
N	2.67191	-1.15448	-0.28204
C	2.39021	2.21004	0.94523
C	2.19808	-2.43465	-0.81958

H	4.80850	-1.54943	-0.35693
H	4.91413	1.06633	0.62318
C	-0.20580	1.61476	-0.85271
O	-0.20654	2.63353	-1.46853
P	-2.58832	-0.09768	0.11638
C	-3.59180	1.47281	0.16495
C	-3.39641	-1.04754	-1.27733
C	-3.17157	-1.03213	1.61833
H	-0.24721	0.87786	1.30805
F	-0.37121	-1.96158	0.47400
H	2.25748	-2.43243	-1.92170
H	2.83295	-3.24400	-0.42589
H	1.15984	-2.57308	-0.47678
H	3.24503	2.63250	1.49458
H	2.13176	2.86786	0.10068
H	1.51979	2.13518	1.61094
H	-4.67304	1.26610	0.22666
H	-3.27964	2.06345	1.04059
H	-3.37913	2.06256	-0.74046
H	-4.25172	-1.24972	1.58019
H	-2.58468	-1.96230	1.65623
H	-2.94197	-0.43830	2.51701
H	-4.48472	-1.15058	-1.12884
H	-3.20337	-0.52665	-2.22867
H	-2.93407	-2.04607	-1.32323

TS (2'-3')_C6F6

SCF (BP86) Energy =	-1468.36413353	
Enthalpy 0K =	-1468.054734	
Enthalpy 298K =	-1468.023283	
Free Energy 298K =	-1468.119187	
Imaginary Frequency =	-546.6273	cm-1
Ru	-1.47130	-0.13149 0.10003
C	-1.24123	1.92270 0.23776
N	-0.87231	2.65647 1.34559
C	-0.88361	4.02413 1.08430
C	-1.26798	4.17173 -0.21853
N	-1.48935	2.88994 -0.71525
C	-0.52360	2.07739 2.64085
C	-1.81674	2.61092 -2.11088
H	-1.39507	5.06247 -0.82815
H	-0.62273	4.76187 1.83852
C	-3.25160	0.01016 -0.38368
O	-4.39209	0.10031 -0.69181
P	-1.69353	-2.47969 0.31929
C	-3.36358	-3.01718 0.96471
C	-1.53548	-3.55968 -1.20136
C	-0.56330	-3.33494 1.53703
H	0.32739	-0.26020 0.42123
H	-1.97845	-0.10133 1.57812
C	1.39525	-0.20852 -0.63553
C	2.18256	-1.39731 -0.57158
C	3.49803	-1.40173 -0.10241
C	2.15469	0.99698 -0.52602
C	4.17154	-0.19327 0.13677
C	3.47079	1.00815 -0.05765
F	1.56511	-2.59565 -0.77556
F	0.39277	-0.19897 -1.67209
F	4.14379	-2.57588 0.06326
F	1.51875	2.18459 -0.69815
F	5.45754	-0.18637 0.55011
F	4.09450	2.18838 0.14911
H	-2.63155	3.27292 -2.44449
H	-0.93258	2.75866 -2.75287
H	-2.14588	1.56548 -2.18554
H	0.16384	2.75893 3.16536
H	-1.42446	1.91661 3.25640
H	-0.03403	1.10757 2.47119

H	-1.69098	-4.62446	-0.95830
H	-2.28810	-3.23971	-1.93958
H	-0.53412	-3.42032	-1.63305
H	-0.83363	-4.39829	1.65206
H	0.47203	-3.25260	1.17853
H	-0.64724	-2.82701	2.51065
H	-3.41707	-4.11299	1.07618
H	-3.53744	-2.53834	1.94109
H	-4.14802	-2.67785	0.27087

TS (5'-6')_C6F6

SCF (BP86) Energy =	-1468.35918913		
Enthalpy 0K =	-1468.046318		
Enthalpy 298K =	-1468.015455		
Free Energy 298K =	-1468.108160		
Imaginary Frequency =	-341.2773	cm-1	
Ru	0.53701	0.85206	-0.13684
C	2.37526	-0.08595	0.15346
N	3.05725	-0.19070	1.34349
C	4.28914	-0.81008	1.16523
C	4.40230	-1.09594	-0.16647
N	3.23083	-0.64713	-0.76911
C	2.52368	0.19453	2.65849
C	2.93711	-0.84181	-2.18843
H	3.35854	-1.80547	-2.51281
H	1.84761	-0.86363	-2.32554
H	3.36123	-0.02879	-2.79935
H	5.19843	-1.57425	-0.73038
H	4.96461	-0.99874	1.99509
H	3.31257	0.03159	3.40767
H	1.62976	-0.42106	2.89409
H	2.25325	1.26251	2.64650
C	1.17939	1.67978	-1.62460
O	1.60523	2.20935	-2.59331
P	-1.28686	2.43357	-0.14241
H	0.03450	-0.10879	1.50558
H	1.20444	2.02043	0.68254
C	-0.63525	-0.85958	0.95141
C	-0.18080	-1.86784	0.04435
C	-1.08500	-2.62354	-0.73739
C	-2.04782	-0.68987	1.00961
C	-2.45856	-2.40436	-0.66063
C	-2.93736	-1.43955	0.25100
F	1.07378	-2.38444	0.13197
F	-0.09163	-1.36138	2.73243
F	-0.59995	-3.59166	-1.54444
F	-2.56207	0.23641	1.86055
F	-3.32141	-3.09067	-1.43797
F	-4.26350	-1.18648	0.32135
C	-3.00567	2.05575	-0.78198
C	-1.61848	3.20434	1.52658
C	-0.89981	3.96403	-1.14207
H	-2.92562	1.68814	-1.81737
H	-3.48494	1.28273	-0.16635
H	-3.62663	2.96729	-0.76820
H	-0.68681	3.67277	1.88081
H	-2.41086	3.96804	1.45429
H	-1.91652	2.42272	2.23782
H	-0.79846	3.70244	-2.20630
H	-1.69994	4.71312	-1.02424
H	0.05528	4.38929	-0.79715

TS (2'-3')_C6F5H_2

SCF (BP86) Energy =	-1369.14490094
Enthalpy 0K =	-1368.827627
Enthalpy 298K =	-1368.797267
Free Energy 298K =	-1368.890671
Imaginary Frequency =	-546.0982 cm-1

Ru	1.27615	0.37865	0.09390
C	1.56664	-1.66584	0.24457
N	1.42866	-2.45576	1.36672
C	1.77596	-3.77976	1.11030
C	2.14401	-3.84137	-0.20416
N	2.02004	-2.55112	-0.71261
C	0.98830	-1.96648	2.67090
C	2.22036	-2.21510	-2.11961
H	2.47346	-4.67841	-0.81416
H	1.73532	-4.54981	1.87620
C	3.01919	0.67760	-0.44804
O	4.13562	0.86876	-0.79665
P	0.92074	2.71084	0.30797
C	2.42161	3.64052	0.92324
C	0.47954	3.71593	-1.20829
C	-0.36070	3.27193	1.54718
H	-0.49718	0.05465	0.45150
H	1.82225	0.48842	1.55551
C	-1.52156	-0.25379	-0.58000
C	-2.57557	0.70635	-0.52452
C	-3.86434	0.39685	-0.07967
C	-1.98230	-1.60284	-0.46410
C	-4.21678	-0.94125	0.15153
C	-3.26027	-1.94709	-0.03200
F	-2.26654	2.01796	-0.73261
F	-0.54804	-0.02379	-1.63180
F	-4.77332	1.38610	0.06647
F	-1.06313	-2.59228	-0.64810
F	-5.47841	-1.24253	0.54421
H	-3.52385	-2.99695	0.11286
H	3.15987	-2.66214	-2.48148
H	1.37667	-2.58016	-2.72830
H	2.28135	-1.12182	-2.20770
H	0.51241	-2.79233	3.22216
H	1.83938	-1.57634	3.25386
H	0.26508	-1.15309	2.51465
H	0.37496	4.78717	-0.96630
H	1.27552	3.58682	-1.95899
H	-0.46438	3.33558	-1.62381
H	-0.35438	4.36963	1.65737
H	-1.35152	2.93913	1.20857
H	-0.13793	2.80370	2.51887
H	2.20933	4.71697	1.03446
H	2.72429	3.22184	1.89583
H	3.25221	3.49921	0.21466

TS (5'-6')_C6F5H_2

SCF (BP86) Energy =	-1369.13902205		
Enthalpy 0K =	-1368.817821		
Enthalpy 298K =	-1368.788187		
Free Energy 298K =	-1368.877634		
Imaginary Frequency =	-267.8262	cm-1	
Ru	0.47582	0.79428	-0.09590
C	2.33416	-0.12450	0.08158
N	3.01948	-0.36058	1.25139
C	4.27146	-0.91042	1.00031
C	4.39491	-1.01816	-0.35658
N	3.20872	-0.53461	-0.90146
C	2.47438	-0.16228	2.60241
C	2.92185	-0.54782	-2.33528
H	3.40292	-1.42810	-2.78858
H	1.83463	-0.61774	-2.47835
H	3.29090	0.36695	-2.82621
H	5.20717	-1.39242	-0.97367
H	4.95312	-1.18175	1.80176
H	3.25477	-0.43619	3.32782
H	1.57595	-0.79763	2.74591
H	2.20869	0.89782	2.74151

C	1.11307	1.83533	-1.44710
O	1.54446	2.50795	-2.32069
P	-1.39885	2.30633	0.07283
H	-0.01536	-0.32866	1.38220
H	1.09137	1.85185	0.89451
C	-0.61983	-1.12121	0.79458
C	-0.09965	-2.09452	-0.11821
C	-0.90434	-2.84472	-0.99164
C	-2.03904	-0.99030	0.74359
C	-2.28209	-2.64563	-1.00136
C	-2.85908	-1.72468	-0.10833
F	1.19441	-2.50237	-0.00153
F	-0.18842	-1.69836	2.52520
H	-0.44922	-3.61052	-1.62307
F	-2.64494	-0.14105	1.61557
F	-3.08304	-3.33259	-1.84866
F	-4.19542	-1.51021	-0.10073
C	-3.07714	1.97284	-0.68839
C	-1.80923	2.82648	1.81982
C	-1.03470	3.97690	-0.68219
H	-2.94376	1.80015	-1.76828
H	-3.53204	1.08037	-0.23861
H	-3.74503	2.83810	-0.53983
H	-0.90779	3.27966	2.26172
H	-2.63171	3.56123	1.82673
H	-2.08942	1.94480	2.41069
H	-0.89096	3.87566	-1.76856
H	-1.86498	4.67544	-0.48719
H	-0.10725	4.37790	-0.24512

TS (2'-3')_C6F5H_3

SCF (BP86) Energy =	-1369.14765826	
Enthalpy 0K =	-1368.830266	
Enthalpy 298K =	-1368.799940	
Free Energy 298K =	-1368.893163	
Imaginary Frequency =	-561.9197	cm-1
Ru	-1.29033	-0.04073 0.08773
C	-0.90395	1.98887 0.23297
N	-0.49190	2.68836 1.34772
C	-0.39541	4.05368 1.09211
C	-0.75326	4.23482 -0.21400
N	-1.06706	2.97556 -0.71844
C	-0.20126	2.07956 2.64361
C	-1.39564	2.72711 -2.11946
H	-0.80463	5.13469 -0.82129
H	-0.08662	4.76658 1.85210
C	-3.04440	0.23655 -0.43415
O	-4.16830	0.41234 -0.76581
P	-1.69666	-2.36416 0.30469
C	-3.41581	-2.77166 0.91598
C	-1.58926	-3.45699 -1.21090
C	-0.65892	-3.29817 1.54622
H	0.47614	-0.30889 0.45511
H	-1.82367	0.03226 1.55521
C	1.57273	-0.33699 -0.59339
C	2.26286	-1.58301 -0.49701
C	3.55950	-1.66587 0.01057
C	2.41081	0.81335 -0.46301
C	4.32275	-0.52157 0.27513
C	3.70763	0.71559 0.04301
F	1.56111	-2.73165 -0.72224
F	0.59590	-0.25919 -1.64557
F	4.09682	-2.89543 0.19935
F	1.86673	2.04173 -0.67043
H	5.34533	-0.59045 0.64621
F	4.39737	1.86213 0.26130
H	-2.15672	3.44710 -2.45994
H	-0.49471	2.81410 -2.74914

H -1.79734 1.70813 -2.20384
H 0.53143 2.70450 3.17731
H -1.11773 1.98624 3.25005
H 0.21405 1.07562 2.47423
H -1.82789 -4.50671 -0.96970
H -2.30108 -3.08411 -1.96459
H -0.57153 -3.39258 -1.62145
H -1.01245 -4.33699 1.65987
H 0.38569 -3.29705 1.20574
H -0.72090 -2.78022 2.51618
H -3.55493 -3.85999 1.02723
H -3.57292 -2.27869 1.88818
H -4.15769 -2.37527 0.20575

TS (5'-6')_C6F5H_3

SCF (BP86) Energy = -1369.14158817
Enthalpy 0K = -1368.820705
Enthalpy 298K = -1368.790969
Free Energy 298K = -1368.880914
Imaginary Frequency = -332.0241 cm-1
Ru -0.25329 -0.84965 -0.07457
C -2.24022 -0.29868 0.22792
N -2.88961 -0.19532 1.43580
C -4.23311 0.11601 1.25988
C -4.44987 0.20123 -0.08700
N -3.22826 -0.05655 -0.70138
C -2.24289 -0.29042 2.75328
C -3.02935 0.01584 -2.14822
H -3.63906 0.83714 -2.55488
H -1.96980 0.22371 -2.34967
H -3.31053 -0.93077 -2.63735
H -5.34972 0.42267 -0.65431
H -4.90653 0.25708 2.10080
H -3.02267 -0.19167 3.52295
H -1.48779 0.51795 2.85688
H -1.75867 -1.27475 2.85524
C -0.78258 -2.02537 -1.35891
O -1.14516 -2.78375 -2.19156
P 1.89147 -1.96326 -0.04848
H 0.08248 0.40427 1.39459
H -0.57998 -1.98681 0.96074
C 0.54683 1.21988 0.73159
C -0.15532 2.00832 -0.23303
C 0.53878 2.84814 -1.13073
C 1.96331 1.36324 0.71692
C 1.92636 2.95051 -1.13587
C 2.62350 2.20217 -0.17162
F -1.49634 2.21473 -0.13868
F -0.03307 1.76620 2.48903
F -0.19851 3.59360 -1.98898
F 2.70110 0.66049 1.61937
H 2.44985 3.59389 -1.84397
F 3.97978 2.24519 -0.13520
C 3.44107 -1.27445 -0.84222
C 2.46962 -2.44930 1.65998
C 1.83588 -3.64333 -0.86585
H 3.22525 -1.04696 -1.89827
H 3.75672 -0.35183 -0.33719
H 4.25644 -2.01555 -0.79010
H 1.69289 -3.08056 2.11958
H 3.41759 -3.01051 1.60756
H 2.60215 -1.54641 2.27038
H 1.62997 -3.53172 -1.94128
H 2.79596 -4.16798 -0.73047
H 1.02603 -4.23944 -0.41784

TS (2'-3')_1,2,3,4-C6F4H2_1

SCF (BP86) Energy = -1269.91601711

Enthalpy 0K = -1269.590616
Enthalpy 298K = -1269.561245
Free Energy 298K = -1269.652223
Imaginary Frequency = -566.6750 cm-1
Ru -1.27860 -0.20223 0.11582
C -1.25204 1.85856 0.22891
N -0.86889 2.64994 1.29284
C -1.01885 4.00516 1.00871
C -1.49887 4.08732 -0.26936
N -1.62970 2.77914 -0.72963
C -0.39353 2.12885 2.57329
C -2.11775 2.41641 -2.06102
H -1.74527 4.94882 -0.88458
H -0.76552 4.78133 1.72603
C -3.04325 -0.27904 -0.43176
O -4.17197 -0.32825 -0.79247
P -1.19627 -2.55661 0.33713
C -2.79072 -3.33253 0.92710
C -0.82748 -3.58514 -1.18144
C 0.01453 -3.24274 1.58330
H 0.51135 -0.08766 0.46298
H -1.82939 -0.21975 1.58398
C 1.50928 0.19847 -0.58304
C 2.48988 -0.83592 -0.53521
C 3.81262 -0.58516 -0.16745
C 2.01572 1.53210 -0.51052
C 4.25564 0.73831 -0.00009
C 3.35078 1.78934 -0.17412
F 2.09204 -2.13395 -0.67554
F 0.48070 -0.01375 -1.61937
F 4.67119 -1.61912 -0.02617
H 1.31712 2.35995 -0.64810
F 5.55518 0.96541 0.32070
H 3.71118 2.81702 -0.07476
H -3.16446 2.07677 -2.01535
H -2.04549 3.29671 -2.71722
H -1.49450 1.60758 -2.46898
H 0.28520 2.86360 3.03278
H -1.23952 1.93092 3.25244
H 0.13981 1.18535 2.38803
H -0.83337 -4.66387 -0.95057
H -1.58922 -3.37015 -1.94768
H 0.15870 -3.29350 -1.57044
H -0.08973 -4.33659 1.68210
H 1.03350 -2.99424 1.25471
H -0.17377 -2.76551 2.55786
H -2.69140 -4.42559 1.03466
H -3.06226 -2.88926 1.89796
H -3.59247 -3.10334 0.20824

TS (5'-6')_1,2,3,4-C6F4H2_1

SCF (BP86) Energy = -1269.91724538
Enthalpy 0K = -1269.588052
Enthalpy 298K = -1269.559410
Free Energy 298K = -1269.646652
Imaginary Frequency = -333.9265 cm-1
Ru 0.58725 0.67269 -0.08057
C 2.39495 -0.36341 0.10188
N 3.05336 -0.67841 1.26803
C 4.25928 -1.31972 1.01235
C 4.38316 -1.41273 -0.34607
N 3.23887 -0.83274 -0.88697
C 2.51486 -0.46452 2.61996
C 2.99306 -0.72872 -2.32538
H 3.47244 -1.58059 -2.83163
H 1.90891 -0.75838 -2.50462
H 3.39487 0.21328 -2.73134
H 5.16959 -1.83438 -0.96616

H	4.90967	-1.66328	1.81206
H	3.29600	-0.73504	3.34581
H	1.61034	-1.09888	2.74586
H	2.25544	0.59914	2.74159
C	1.27625	1.73907	-1.38633
O	1.72716	2.42063	-2.24316
P	-1.24429	2.20587	0.14343
H	0.03389	-0.54743	1.34713
H	1.23502	1.68339	0.95289
C	-0.64784	-1.14216	0.63587
C	-0.21399	-1.76779	-0.57436
C	-1.15296	-2.33097	-1.48212
C	-2.05024	-1.08680	0.86512
C	-2.50877	-2.25456	-1.21451
C	-2.96191	-1.63988	-0.02084
H	0.83441	-2.04306	-0.68222
F	0.03601	-2.05705	2.23409
H	-0.81490	-2.86432	-2.37454
F	-2.52889	-0.45000	1.96520
F	-3.43583	-2.76940	-2.05817
F	-4.28785	-1.52214	0.21476
C	-2.95025	1.89832	-0.56408
C	-1.62781	2.64154	1.91809
C	-0.88232	3.89582	-0.56370
H	-2.85873	1.66903	-1.63745
H	-3.42297	1.04368	-0.06002
H	-3.58550	2.79074	-0.43435
H	-0.71453	3.04207	2.38481
H	-2.43284	3.39350	1.97241
H	-1.93192	1.73080	2.45235
H	-0.76228	3.82566	-1.65559
H	-1.69884	4.59821	-0.32894
H	0.06044	4.26891	-0.13469

TS(2'-3')_1,2,3,4-C6F4H2_2

SCF (BP86) Energy =	-1269.92184728		
Enthalpy 0K =	-1269.596452		
Enthalpy 298K =	-1269.567162		
Free Energy 298K =	-1269.657951		
Imaginary Frequency =	-559.1485	cm-1	
Ru	0.82444	0.77652	0.08056
C	1.98520	-0.92944	0.24496
N	2.22069	-1.68016	1.37766
C	3.11075	-2.72192	1.12910
C	3.45357	-2.63854	-0.19097
N	2.77063	-1.54214	-0.71059
C	1.62339	-1.41181	2.68354
C	2.78121	-1.18091	-2.12544
H	4.10980	-3.25677	-0.79795
H	3.42109	-3.41814	1.90382
C	2.24940	1.80141	-0.50461
O	3.16184	2.45810	-0.88009
P	-0.51636	2.71906	0.28228
C	0.43333	4.22407	0.85579
C	-1.37826	3.39979	-1.23318
C	-1.89420	2.68171	1.54401
H	-0.61364	-0.27970	0.49071
H	1.29019	1.14013	1.52897
C	-1.41995	-1.02703	-0.52847
C	-2.78538	-0.62713	-0.44061
C	-3.77763	-1.47580	0.05754
C	-1.22786	-2.43879	-0.38543
C	-3.51857	-2.82453	0.32006
C	-2.21016	-3.29516	0.09558
F	-3.09249	0.68244	-0.67441
F	-0.67016	-0.40718	-1.59943
F	-5.02297	-0.96534	0.23078
F	0.03061	-2.91819	-0.60867

H	-4.31731	-3.47542	0.67923
H	-1.95336	-4.34672	0.24990
H	3.81442	-1.19382	-2.50722
H	2.16083	-1.88201	-2.70785
H	2.36967	-0.16734	-2.22591
H	1.57704	-2.35101	3.25632
H	2.21525	-0.66785	3.24264
H	0.60962	-1.01420	2.53109
H	-1.93654	4.32247	-1.00069
H	-0.61897	3.61542	-2.00179
H	-2.06772	2.63606	-1.62002
H	-2.36874	3.67254	1.64514
H	-2.64292	1.94218	1.22835
H	-1.47331	2.37476	2.51439
H	-0.22817	5.10007	0.96209
H	0.90453	3.99797	1.82516
H	1.23031	4.44895	0.13038

TS(5'-6')_1,2,3,4-C6F4H2_2

SCF (BP86) Energy =	-1269.91469673		
Enthalpy 0K =	-1269.585662		
Enthalpy 298K =	-1269.556977		
Free Energy 298K =	-1269.644487		
Imaginary Frequency =	-280.1795 cm-1		
Ru	0.23467	0.75915	-0.02801
C	2.22546	0.17873	0.14681
N	2.89710	-0.11132	1.31175
C	4.23903	-0.37887	1.06630
C	4.43302	-0.24533	-0.28017
N	3.19890	0.09668	-0.82520
C	2.27209	-0.23351	2.63722
C	2.97270	0.25987	-2.26048
H	3.61790	-0.44439	-2.80785
H	1.92098	0.03014	-2.48110
H	3.19197	1.28956	-2.58591
H	5.32445	-0.36433	-0.88997
H	4.92819	-0.64678	1.86245
H	3.06164	-0.47478	3.36435
H	1.50419	-1.03544	2.62018
H	1.80646	0.72541	2.91543
C	0.73844	2.13042	-1.11414
O	1.08977	3.01821	-1.81405
P	-1.91746	1.83303	0.20099
H	-0.08608	-0.67789	1.21501
H	0.56698	1.70969	1.17870
C	-0.50313	-1.45971	0.47445
C	0.23591	-2.17314	-0.52501
C	-0.37565	-2.91202	-1.54689
C	-1.91543	-1.58836	0.34628
C	-1.77137	-2.98327	-1.64257
C	-2.52778	-2.32246	-0.66644
F	1.58396	-2.32434	-0.38379
F	-0.02050	-2.19351	2.14662
H	0.26697	-3.46623	-2.23613
F	-2.71007	-1.00380	1.28524
H	-2.27211	-3.54746	-2.43183
F	-3.88665	-2.35413	-0.70226
C	-3.44927	1.29309	-0.73052
C	-2.51202	1.99701	1.96444
C	-1.86847	3.63654	-0.28920
H	-3.22451	1.30569	-1.80897
H	-3.73666	0.27432	-0.43879
H	-4.28528	1.98320	-0.52623
H	-1.74613	2.54766	2.53322
H	-3.46747	2.54633	2.00628
H	-2.63300	0.99901	2.40505
H	-1.65307	3.72851	-1.36458
H	-2.83368	4.12104	-0.06767

H -1.06701 4.14375 0.26976

TS(2'-3')_1,2,3,5-C6F4H2_1

SCF (BP86) Energy = -1269.92485040
Enthalpy 0K = -1269.599399
Enthalpy 298K = -1269.570085
Free Energy 298K = -1269.661040
Imaginary Frequency = -577.7690 cm⁻¹

Ru -1.23615 0.14591 0.11356
C -0.51690 2.07856 0.22272
N 0.13602 2.68742 1.27520
C 0.44942 4.01408 0.99041
C -0.00358 4.26123 -0.27607
N -0.58183 3.07776 -0.72922
C 0.44106 2.02908 2.54440
C -1.19774 2.91336 -2.04659
H 0.04521 5.15773 -0.88862
H 0.97154 4.65297 1.69767
C -2.93317 0.66869 -0.40799
O -4.02002 1.00097 -0.74606
P -1.94426 -2.10141 0.33171
C -3.70003 -2.30265 0.93916
C -1.95640 -3.18410 -1.19393
C -1.01924 -3.16028 1.56110
H 0.47056 -0.35426 0.46883
H -1.73855 0.30695 1.58881
C 1.53027 -0.40865 -0.59789
C 2.10117 -1.71385 -0.53163
C 3.41563 -1.90224 -0.10622
C 2.43911 0.68758 -0.48737
C 4.28864 -0.82755 0.11320
C 3.75332 0.45170 -0.09045
F 1.29247 -2.80105 -0.70651
F 0.51298 -0.25763 -1.63097
F 3.85840 -3.17279 0.05496
H 2.08393 1.70887 -0.62974
H 5.32235 -0.98629 0.42013
F 4.57196 1.52555 0.08224
H -2.29490 2.98377 -1.97856
H -0.81964 3.70039 -2.71624
H -0.92584 1.92938 -2.45462
H 1.34082 2.48803 2.98169
H -0.40342 2.12612 3.24692
H 0.61848 0.96188 2.34831
H -2.32247 -4.19966 -0.96669
H -2.60839 -2.72042 -1.95123
H -0.93299 -3.23887 -1.59224
H -1.48482 -4.15539 1.66146
H 0.01917 -3.26789 1.21745
H -1.02282 -2.65177 2.53800
H -3.97003 -3.36662 1.04513
H -3.79736 -1.79850 1.91340
H -4.38713 -1.81588 0.22990

TS(5'-6')_1,2,3,5-C6F4H2_1

SCF (BP86) Energy = -1269.92595059
Enthalpy 0K = -1269.597035
Enthalpy 298K = -1269.568349
Free Energy 298K = -1269.655904
Imaginary Frequency = -396.0784 cm⁻¹

Ru 0.39429 0.72906 -0.05727
C 2.32098 -0.02311 0.25786
N 2.96096 -0.18546 1.46423
C 4.25269 -0.66746 1.29183
C 4.45075 -0.80860 -0.05362
N 3.26516 -0.41869 -0.67033
C 2.33173 0.00513 2.77953
C 3.07847 -0.41255 -2.12210

H 3.71801 -1.19088 -2.56522
H 2.02646 -0.63309 -2.35122
H 3.34017 0.56721 -2.55224
H 5.31506 -1.14728 -0.61842
H 4.90526 -0.88003 2.13416
H 3.11089 -0.09296 3.54990
H 1.53894 -0.76414 2.90327
H 1.89478 1.01514 2.82754
C 0.98464 1.83263 -1.37759
O 1.36791 2.53771 -2.24799
P -1.64882 1.98130 0.01366
H -0.05409 -0.55180 1.41494
H 0.83327 1.86670 0.95565
C -0.62548 -1.20584 0.66584
C -0.03285 -1.74393 -0.52168
C -0.85913 -2.41803 -1.45155
C -2.02485 -1.36631 0.83530
C -2.22766 -2.57819 -1.28717
C -2.78767 -2.04244 -0.10705
H 1.04071 -1.91876 -0.57636
F 0.18534 -1.98690 2.31079
F -0.25772 -2.96212 -2.54251
F -2.64668 -0.80705 1.90843
H -2.84723 -3.10490 -2.01417
F -4.12900 -2.11403 0.07781
C -3.24476 1.42046 -0.78799
C -2.20209 2.38040 1.75120
C -1.48520 3.69497 -0.70971
H -3.05232 1.18419 -1.84634
H -3.62513 0.51798 -0.28923
H -4.00540 2.21670 -0.72356
H -1.38619 2.91219 2.26481
H -3.10683 3.01110 1.73956
H -2.40852 1.44157 2.28370
H -1.28511 3.62690 -1.78996
H -2.40612 4.27743 -0.54298
H -0.63426 4.20419 -0.23145

TS(2'-3')_1,2,3,5-C6F4H2_2

SCF (BP86) Energy = -1269.92488341
Enthalpy 0K = -1269.599728
Enthalpy 298K = -1269.570417
Free Energy 298K = -1269.661460
Imaginary Frequency = -540.1621 cm⁻¹

Ru -1.18986 -0.04805 0.09174
C -0.79802 1.97902 0.24299
N -0.42559 2.68286 1.36924
C -0.31677 4.04712 1.11142
C -0.62547 4.22277 -0.20800
N -0.92381 2.96202 -0.71797
C -0.18856 2.07912 2.67812
C -1.19511 2.70565 -2.12976
H -0.65407 5.12017 -0.82049
H -0.03792 4.76321 1.87999
C -2.92392 0.23549 -0.48322
O -4.03504 0.41682 -0.85441
P -1.61759 -2.36674 0.30722
C -3.35100 -2.75780 0.88893
C -1.49289 -3.46666 -1.20202
C -0.61180 -3.30690 1.57105
H 0.59623 -0.32138 0.46834
H -1.77018 0.03475 1.54302
C 1.66321 -0.36362 -0.53825
C 2.36906 -1.60309 -0.46737
C 3.69449 -1.73077 -0.05862
C 2.53211 0.76861 -0.44411
C 4.43785 -0.56302 0.14957
C 3.86266 0.69988 -0.03619

F 1.63936 -2.74279 -0.67420
F 0.66643 -0.28057 -1.60385
H 4.14182 -2.72066 0.05139
F 1.97380 1.99663 -0.64105
F 5.74170 -0.65672 0.52421
H 4.44506 1.61540 0.08599
H -1.90883 3.45130 -2.51442
H -0.26236 2.74645 -2.71615
H -1.63348 1.70253 -2.22058
H 0.52573 2.70319 3.23741
H -1.12836 1.99265 3.24888
H 0.22798 1.07231 2.52976
H -1.74484 -4.51358 -0.96200
H -2.18802 -3.08987 -1.96924
H -0.46763 -3.41069 -1.59449
H -0.97249 -4.34413 1.67769
H 0.43968 -3.30941 1.25248
H -0.69168 -2.78816 2.53932
H -3.50214 -3.84447 1.00124
H -3.52124 -2.25964 1.85626
H -4.07611 -2.35712 0.16392

TS (5'-6')_1,2,3,5-C6F4H2_2

SCF (BP86) Energy = -1269.91780787
Enthalpy 0K = -1269.588993
Enthalpy 298K = -1269.560271
Free Energy 298K = -1269.648025
Imaginary Frequency = -248.4183 cm-1
Ru -0.11314 -0.79818 -0.11635
C -2.13687 -0.37089 0.08848
N -2.83828 -0.33129 1.27276
C -4.19307 -0.11253 1.05033
C -4.36520 -0.02157 -0.30236
N -3.10538 -0.18142 -0.87358
C -2.23326 -0.39691 2.61043
C -2.85827 -0.07634 -2.31106
H -3.57334 0.63946 -2.74475
H -1.83590 0.29435 -2.46860
H -2.96725 -1.05284 -2.80950
H -5.25723 0.14267 -0.90065
H -4.90608 -0.03292 1.86637
H -3.04055 -0.32002 3.35393
H -1.51075 0.43327 2.74496
H -1.71662 -1.36178 2.73650
C -0.46001 -1.90157 -1.52418
O -0.69361 -2.62221 -2.43497
P 2.04635 -1.84676 0.06558
H 0.14365 0.36124 1.36769
H -0.46684 -2.00817 0.83135
C 0.48334 1.32152 0.80459
C -0.33274 2.15875 -0.02448
C 0.17858 3.11257 -0.91813
C 1.88249 1.57245 0.64071
C 1.55924 3.26965 -1.01273
C 2.43454 2.51625 -0.21676
F -1.67445 2.20836 0.19790
F 0.04600 1.72422 2.54655
H -0.50695 3.74725 -1.48291
F 2.73427 0.88574 1.45854
F 2.07364 4.18047 -1.87876
H 3.51518 2.66400 -0.25970
C 3.60473 -1.19094 -0.73793
C 2.58395 -2.18733 1.82214
C 2.03803 -3.58702 -0.61592
H 3.42175 -1.06732 -1.81693
H 3.85542 -0.21480 -0.30180
H 4.44489 -1.88938 -0.58646
H 1.80451 -2.79663 2.30623

H 3.54229 -2.73302 1.84112
H 2.68098 -1.23820 2.36545
H 1.86020 -3.56418 -1.70175
H 3.00000 -4.08599 -0.41314
H 1.22193 -4.15471 -0.14286

TS (2'-3')_1,2,3,5-C6F4H2_5

SCF (BP86) Energy = -1269.91619725
Enthalpy 0K = -1269.591371
Enthalpy 298K = -1269.561802
Free Energy 298K = -1269.654219
Imaginary Frequency = -528.0103 cm-1
Ru -1.40377 -0.08681 0.08628
C -1.01613 1.94264 0.20645
N -0.46638 2.63206 1.26900
C -0.35139 3.99300 0.99766
C -0.82820 4.18267 -0.26945
N -1.22702 2.93211 -0.73565
C -0.08227 2.01710 2.53892
C -1.75171 2.70203 -2.08033
H -0.91003 5.08279 -0.87316
H 0.05744 4.69675 1.71802
C -3.19115 0.11758 -0.36035
O -4.34095 0.23367 -0.62234
P -1.63792 -2.42046 0.29862
C -3.27799 -3.02017 0.95981
C -1.45613 -3.49042 -1.22943
C -0.44840 -3.22975 1.49105
H 0.36308 -0.32178 0.42495
H -1.88922 -0.03189 1.57686
C 1.38636 -0.26808 -0.61242
C 2.09617 -1.50937 -0.65452
C 3.44832 -1.54362 -0.31987
C 2.15066 0.93130 -0.45327
C 4.18335 -0.38003 -0.04302
C 3.50004 0.84577 -0.12395
H 1.58373 -2.44218 -0.89418
F 0.33848 -0.17462 -1.65590
F 4.09714 -2.73351 -0.28988
H 1.67197 1.91023 -0.50184
F 5.49511 -0.43523 0.28921
F 4.20235 1.98263 0.10876
H -2.63676 3.33461 -2.25639
H -0.98178 2.92493 -2.83709
H -2.04015 1.64520 -2.15709
H 0.69001 2.63784 3.01797
H -0.95381 1.92736 3.20822
H 0.31371 1.01159 2.33703
H -1.55277 -4.56291 -0.98998
H -2.23713 -3.20452 -1.95210
H -0.47643 -3.30485 -1.69629
H -0.59134 -4.32271 1.53181
H 0.58540 -3.00132 1.18724
H -0.61645 -2.79905 2.49068
H -3.29410 -4.11738 1.06822
H -3.45640 -2.54853 1.93871
H -4.07982 -2.70369 0.27476

TS (5'-6')_1,2,3,5-C6F4H2_5

SCF (BP86) Energy = -1269.91794299
Enthalpy 0K = -1269.589512
Enthalpy 298K = -1269.560546
Free Energy 298K = -1269.649521
Imaginary Frequency = -361.3943 cm-1
Ru 0.55658 0.73230 -0.06724
C 2.35600 -0.32006 0.13109
N 3.12299 -0.45109 1.26469
C 4.27955 -1.17860 1.01317

C	4.26110	-1.51398	-0.31217
N	3.08205	-0.99046	-0.83528
C	2.72499	0.00858	2.60332
C	2.70438	-1.11595	-2.24371
H	3.11386	-2.05782	-2.63945
H	1.60854	-1.13433	-2.32262
H	3.09016	-0.27026	-2.83508
H	4.96946	-2.07031	-0.92000
H	4.99889	-1.40507	1.79538
H	3.57622	-0.14035	3.28415
H	1.83749	-0.58084	2.92272
H	2.47625	1.08074	2.55674
C	1.14395	1.55390	-1.58177
O	1.51908	2.07976	-2.57437
P	-1.23754	2.30427	0.01226
H	0.10223	-0.26268	1.60176
H	1.30666	1.88111	0.73237
C	-0.68831	-0.86997	1.03356
C	-0.36225	-1.61766	-0.14361
C	-1.40901	-2.22507	-0.87736
C	-2.05290	-0.75883	1.43370
C	-2.74088	-2.11376	-0.49726
C	-3.03212	-1.39580	0.69022
H	0.64332	-2.00216	-0.31192
F	0.24972	-1.59093	2.66628
F	-1.09758	-2.97253	-1.96308
H	-2.33218	-0.22044	2.34015
F	-3.73586	-2.68995	-1.20721
F	-4.33495	-1.28839	1.04410
C	-2.88060	1.98314	-0.82107
C	-1.75370	2.82521	1.73154
C	-0.78840	3.96256	-0.71897
H	-2.70332	1.79300	-1.89149
H	-3.34991	1.09227	-0.37921
H	-3.55586	2.84822	-0.71011
H	-0.86779	3.20781	2.26174
H	-2.52524	3.61184	1.68607
H	-2.14824	1.96187	2.28618
H	-0.56155	3.84539	-1.78964
H	-1.61145	4.68523	-0.59454
H	0.11526	4.33812	-0.21421

TS(2'-3')_1,2,4,5-C6F4H2_1

SCF (BP86) Energy =	-1269.92191860	
Enthalpy 0K =	-1269.596743	
Enthalpy 298K =	-1269.567365	
Free Energy 298K =	-1269.658658	
Imaginary Frequency =	-566.8293 cm ⁻¹	
Ru	-1.28017	0.26032 0.11889
C	-0.27253	2.05925 0.23378
N	0.46033	2.56162 1.29029
C	0.97638	3.82384 1.00719
C	0.57511	4.13602 -0.26233
N	-0.17604	3.05539 -0.71893
C	0.64929	1.86835 2.56340
C	-0.79894	2.98407 -2.04144
H	0.76549	5.01350 -0.87481
H	1.58597	4.37568 1.71776
C	-2.87267	1.03334 -0.41747
O	-3.89315	1.52585 -0.76752
P	-2.31799	-1.85389 0.33234
C	-4.09138	-1.79574 0.91853
C	-2.46796	-2.93172 -1.18955
C	-1.57037	-3.03134 1.57496
H	0.34415	-0.49706 0.46517
H	-1.76698	0.50299 1.58941
C	1.36498	-0.70639 -0.58492
C	1.76836	-2.07468 -0.52984

C	3.05323	-2.47312	-0.17662
C	2.42751	0.24483	-0.51321
C	4.05096	-1.50480	-0.00385
C	3.72105	-0.15153	-0.17635
F	0.80101	-3.03199	-0.68747
F	0.35941	-0.41373	-1.61847
H	3.28571	-3.53503	-0.06745
H	2.21593	1.30728	-0.64516
F	5.31839	-1.86436	0.32102
F	4.69359	0.78595	-0.04381
H	-1.87861	3.19216	-1.97778
H	-0.32019	3.72495	-2.69916
H	-0.65086	1.97827	-2.46022
H	1.62284	2.15405	2.99032
H	-0.15593	2.12628	3.27151
H	0.62205	0.78550	2.37463
H	-2.97869	-3.88297	-0.96295
H	-3.03747	-2.38383	-1.95704
H	-1.45771	-3.13367	-1.57389
H	-2.17577	-3.94843	1.67336
H	-0.55491	-3.28858	1.24213
H	-1.50962	-2.52338	2.55023
H	-4.51628	-2.80855	1.01821
H	-4.12581	-1.28359	1.89286
H	-4.69043	-1.21248	0.20225

TS(5'-6')_1,2,4,5-C6F4H2_1

SCF (BP86) Energy =	-1269.92318610		
Enthalpy 0K =	-1269.594491		
Enthalpy 298K =	-1269.565723		
Free Energy 298K =	-1269.653612		
Imaginary Frequency =	-365.7885 cm-1		
Ru	0.44018	0.76655	-0.07809
C	2.30622	-0.16750	0.12718
N	3.04676	-0.30643	1.27713
C	4.26057	-0.93345	1.02590
C	4.30712	-1.19311	-0.31570
N	3.10903	-0.72688	-0.84936
C	2.57558	0.04465	2.62519
C	2.78858	-0.79396	-2.27583
H	3.24475	-1.70029	-2.70259
H	1.69774	-0.84446	-2.39783
H	3.16518	0.09365	-2.80904
H	5.07271	-1.66129	-0.92841
H	4.97063	-1.15221	1.81871
H	3.41975	-0.06304	3.32235
H	1.73831	-0.63858	2.88754
H	2.23166	1.09110	2.62518
C	1.04334	1.73125	-1.49639
O	1.44171	2.34943	-2.42446
P	-1.49678	2.16411	-0.04566
H	0.04454	-0.35906	1.51812
H	1.05328	1.91430	0.82445
C	-0.67485	-1.01719	0.91927
C	-0.32698	-1.67716	-0.29840
C	-1.32025	-2.35655	-1.04175
C	-2.03850	-1.08566	1.32339
C	-2.64135	-2.39966	-0.61047
C	-3.00301	-1.76969	0.60142
H	0.71269	-1.91383	-0.52427
F	0.27863	-1.78819	2.49317
F	-0.95963	-3.01136	-2.17320
F	-2.40138	-0.46496	2.47964
F	-3.58027	-3.05879	-1.33208
H	-4.03632	-1.81341	0.95394
C	-3.02902	1.64153	-0.97728
C	-2.15722	2.60104	1.64325
C	-1.20494	3.86665	-0.75370

H -2.77054 1.53328 -2.04272
H -3.36673 0.66397 -0.60082
H -3.83847 2.38288 -0.86899
H -1.35322 3.09594 2.21051
H -3.02133 3.28125 1.55982
H -2.44759 1.68409 2.17390
H -0.91988 3.78752 -1.81371
H -2.11066 4.48827 -0.66165
H -0.37496 4.34019 -0.20644

TS (2'-3')_1,2,3-C6F3H3_1

SCF (BP86) Energy = -1170.69191816
Enthalpy 0K = -1170.358484
Enthalpy 298K = -1170.330103
Free Energy 298K = -1170.418854
Imaginary Frequency = -570.6089 cm⁻¹

Ru 0.89538 0.61132 0.10739
C 1.76894 -1.25446 0.22840
N 1.78092 -2.12255 1.30121
C 2.50225 -3.28033 1.02052
C 2.95564 -3.15852 -0.26409
N 2.49886 -1.92847 -0.73156
C 1.13739 -1.84839 2.58482
C 2.76351 -1.40380 -2.07194
H 3.54505 -3.83331 -0.87941
H 2.61979 -4.08220 1.74462
C 2.44619 1.44207 -0.46422
O 3.43813 1.97365 -0.83870
P -0.19651 2.69972 0.32431
C 0.91039 4.08951 0.90412
C -0.97970 3.46416 -1.19311
C -1.57842 2.80064 1.57687
H -0.65802 -0.25854 0.48914
H 1.39806 0.87788 1.56882
C -1.45043 -0.95757 -0.55430
C -2.77646 -0.44034 -0.49191
C -3.84748 -1.23691 -0.08532
C -1.32908 -2.37859 -0.45278
C -3.70266 -2.61529 0.11649
C -2.42282 -3.16549 -0.07981
F -2.97288 0.90179 -0.66034
F -0.62300 -0.33845 -1.60140
F -5.05930 -0.64410 0.06416
H -0.34387 -2.82588 -0.60300
H -4.56827 -3.21633 0.40159
H -2.28094 -4.24519 0.03503
H 3.56217 -0.64577 -2.04560
H 3.06785 -2.23565 -2.72479
H 1.84639 -0.94660 -2.47042
H 0.87094 -2.80215 3.06535
H 1.81084 -1.27653 3.24474
H 0.23215 -1.25224 2.40039
H -1.43610 4.44195 -0.96364
H -0.20346 3.59385 -1.96399
H -1.74750 2.77576 -1.57457
H -1.95358 3.83336 1.67663
H -2.39258 2.13797 1.25148
H -1.19863 2.45100 2.54974
H 0.34978 5.03318 1.01123
H 1.35119 3.80988 1.87381
H 1.72913 4.22625 0.18086

TS (5'-6')_1,2,3-C6F3H3_1

SCF (BP86) Energy = -1170.69169766
Enthalpy 0K = -1170.354647
Enthalpy 298K = -1170.326936
Free Energy 298K = -1170.412130
Imaginary Frequency = -348.0071 cm⁻¹

Ru 0.38557 0.64565 -0.00287
C 2.30792 -0.16361 0.14774
N 2.93166 -0.61338 1.28819
C 4.23080 -1.03000 1.02494
C 4.45088 -0.83620 -0.31051
N 3.27065 -0.31405 -0.83254
C 2.28416 -0.74625 2.60210
C 3.10236 0.04267 -2.24117
H 3.72835 -0.62301 -2.85507
H 2.04663 -0.08841 -2.51810
H 3.39070 1.09012 -2.42416
H 5.32689 -1.02144 -0.92620
H 4.87290 -1.43788 1.80078
H 3.05001 -1.04903 3.33155
H 1.47766 -1.50789 2.52089
H 1.86254 0.22766 2.89740
C 1.00573 2.04373 -0.99129
O 1.41527 2.94290 -1.64397
P -1.66526 1.84513 0.33404
H -0.07670 -0.91200 1.10226
H 0.79912 1.48773 1.27141
C -0.62736 -1.42075 0.22958
C -0.03732 -1.72162 -1.03920
C -0.84154 -2.19353 -2.10954
C -2.03082 -1.59903 0.34824
C -2.21689 -2.36129 -1.96589
C -2.79321 -2.06500 -0.71341
H 1.04560 -1.82044 -1.11115
F 0.12685 -2.54164 1.67178
H -0.35901 -2.47013 -3.05253
F -2.65517 -1.27101 1.51176
H -2.85517 -2.72793 -2.77338
F -4.13715 -2.16896 -0.54646
C -3.25920 1.46602 -0.57168
C -2.22151 1.85750 2.11625
C -1.51182 3.67618 -0.00064
H -3.06648 1.46749 -1.65603
H -3.63531 0.47474 -0.28245
H -4.02248 2.22637 -0.33478
H -1.40987 2.27307 2.73341
H -3.13178 2.46800 2.23974
H -2.41913 0.82428 2.43364
H -1.31398 3.84457 -1.07030
H -2.43582 4.20318 0.28877
H -0.66312 4.07586 0.57558

TS (2'-3')_1,2,3-C6F3H3_2

SCF (BP86) Energy = -1170.69517273
Enthalpy 0K = -1170.361863
Enthalpy 298K = -1170.333549
Free Energy 298K = -1170.421915
Lowest Frequency = -554.1961 cm⁻¹

Ru 0.39758 -0.89783 0.07621
C -1.64073 -1.22003 0.23359
N -2.41961 -1.13927 1.36898
C -3.74255 -1.49024 1.11198
C -3.81452 -1.80261 -0.21627
N -2.53125 -1.64350 -0.73236
C -1.92085 -0.74589 2.68436
C -2.21109 -1.76487 -2.15189
H -4.65458 -2.11498 -0.83110
H -4.50428 -1.49175 1.88722
C 0.71420 -2.60625 -0.55749
O 0.91745 -3.70070 -0.96546
P 2.72575 -0.52386 0.28997
C 3.67903 -2.04092 0.82543
C 3.71459 0.00403 -1.20914
C 3.27963 0.70310 1.58618

H	0.05330	0.85179	0.52186
H	0.52541	-1.51632	1.50852
C	-0.27139	1.90708	-0.46625
C	0.66227	2.98180	-0.35471
C	0.33291	4.24826	0.11626
C	-1.62957	2.33668	-0.34097
C	-1.01413	4.57096	0.35923
C	-1.99867	3.59330	0.12883
F	1.97938	2.68145	-0.59286
F	-0.01996	0.97591	-1.55703
H	1.13601	4.97906	0.24725
F	-2.59742	1.40256	-0.57785
H	-1.29203	5.56830	0.70800
H	-3.06358	3.80265	0.26520
H	-2.69067	-2.66554	-2.56674
H	-2.55391	-0.87331	-2.70248
H	-1.12097	-1.85348	-2.25413
H	-2.74926	-0.31445	3.26748
H	-1.50256	-1.61253	3.22325
H	-1.12664	0.00259	2.54935
H	4.78659	0.10910	-0.97037
H	3.58827	-0.75484	-1.99780
H	3.31802	0.96278	-1.57215
H	4.37828	0.70859	1.68756
H	2.92697	1.70249	1.29645
H	2.82249	0.42628	2.54921
H	4.75379	-1.82119	0.93938
H	3.27112	-2.39552	1.78498
H	3.54224	-2.83800	0.07848

TS (5'-6')_1,2,3-C6F3H3_2

SCF (BP86) Energy =	-1170.68685937
Enthalpy 0K =	-1170.350046
Enthalpy 298K =	-1170.322244
Free Energy 298K =	-1170.408014
Imaginary Frequency =	-263.6120 cm ⁻¹
Ru	0.08290 -0.67162 -0.04274
C	-1.97902 -0.57733 0.20311
N	-2.64725 -0.40990 1.39475
C	-4.02361 -0.49094 1.21694
C	-4.24112 -0.72661 -0.11167
N	-2.98724 -0.77785 -0.71476
C	-2.00989 -0.07414 2.67605
C	-2.79559 -0.94296 -2.15495
H	-3.63804 -0.47152 -2.68399
H	-1.86146 -0.44345 -2.44735
H	-2.73634 -2.00765 -2.43243
H	-5.16166 -0.85736 -0.67395
H	-4.71987 -0.36583 2.04169
H	-2.80137 0.02714 3.43353
H	-1.44423 0.87618 2.58440
H	-1.32684 -0.88565 2.97413
C	-0.09620 -2.12618 -1.12468
O	-0.22401 -3.07419 -1.82335
P	2.41284 -1.23546 0.19379
H	0.15005 0.82513 1.14020
H	0.00032 -1.66108 1.17927
C	0.28721 1.67722 0.36355
C	-0.70070 2.16528 -0.55171
C	-0.40142 2.98539 -1.64847
C	1.60503 2.14147 0.06115
C	0.91819 3.38297 -1.89020
C	1.93232 2.96813 -1.00582
F	-2.02112 1.99992 -0.25605
F	-0.17755 2.33455 2.04433
H	-1.23235 3.33833 -2.26558
F	2.59826 1.79926 0.93921
H	1.15654 4.02605 -2.74135

H	2.97127	3.28642	-1.12686
C	3.78139	-0.48815	-0.84148
C	3.06375	-1.08490	1.93846
C	2.72934	-3.05194	-0.11446
H	3.54131	-0.63737	-1.90597
H	3.84461	0.58834	-0.63447
H	4.74859	-0.96671	-0.61306
H	2.43751	-1.71197	2.59253
H	4.11169	-1.42389	1.99732
H	2.98658	-0.04041	2.26751
H	2.51758	-3.29713	-1.16626
H	3.77716	-3.30578	0.11629
H	2.05788	-3.64831	0.52241

TS (2'-3')_1,2,4-C6F3H3_1

SCF (BP86) Energy =	-1170.69474516
Enthalpy 0K =	-1170.361449
Enthalpy 298K =	-1170.333123
Free Energy 298K =	-1170.421732
Imaginary Frequency =	-564.7394 cm ⁻¹
Ru	-1.13570 0.10445 0.11639
C	-0.45159 2.04810 0.22910
N	0.14740 2.68428 1.29749
C	0.44413 4.01371 1.00653
C	0.03673 4.23407 -0.28041
N	-0.49870 3.03271 -0.73890
C	0.41087 2.04881 2.58727
C	-1.05270 2.83096 -2.07849
H	0.08971 5.12357 -0.90281
H	0.92140 4.67402 1.72580
C	-2.82717 0.59666 -0.44625
O	-3.90908 0.91234 -0.81627
P	-1.81178 -2.15129 0.33270
C	-3.57383 -2.37828 0.91307
C	-1.78235 -3.24008 -1.18825
C	-0.89156 -3.19264 1.58142
H	0.59881 -0.35941 0.47347
H	-1.67626 0.26594 1.58044
C	1.63732 -0.40729 -0.55415
C	2.24925 -1.69573 -0.50653
C	3.58391 -1.89715 -0.17262
C	2.54296 0.69465 -0.48465
C	4.40720 -0.77402 -0.00748
C	3.89669 0.51812 -0.16893
F	1.44029 -2.79029 -0.66579
F	0.59401 -0.27722 -1.60234
H	3.97838 -2.91150 -0.07822
H	2.14157 1.70187 -0.61944
F	5.72248 -0.95470 0.29823
H	4.56341 1.37976 -0.07552
H	-2.15373 2.84928 -2.05393
H	-0.68641 3.63174 -2.73835
H	-0.71689 1.85834 -2.46625
H	1.28503 2.52782 3.05433
H	-0.46262 2.14169 3.25406
H	0.61186 0.98179 2.41391
H	-2.13382 -4.26138 -0.96352
H	-2.43049 -2.78991 -1.95691
H	-0.75193 -3.27593 -1.57010
H	-1.34011 -4.19634 1.67468
H	0.15502 -3.28009 1.25742
H	-0.92312 -2.68298 2.55725
H	-3.82997 -3.44583 1.01805
H	-3.69433 -1.87249 1.88388
H	-4.25639 -1.90366 0.19127

TS (5'-6')_1,2,4-C6F3H3_1

SCF (BP86) Energy =	-1170.69544408
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Enthalpy 0K = -1170.358605
Enthalpy 298K = -1170.330860
Free Energy 298K = -1170.416434
Imaginary Frequency = -325.2411 cm⁻¹
Ru 0.38597 0.69494 -0.00873
C 2.27955 -0.20170 0.06094
N 2.98608 -0.56654 1.18282
C 4.23528 -1.07624 0.85237
C 4.34011 -1.02847 -0.51004
N 3.14077 -0.49951 -0.97875
C 2.45517 -0.53885 2.55409
C 2.86995 -0.26182 -2.39640
H 3.37110 -1.03996 -2.99262
H 1.78524 -0.31237 -2.56602
H 3.23143 0.73092 -2.70943
H 5.14705 -1.31980 -1.17694
H 4.92698 -1.43955 1.60748
H 3.27770 -0.77780 3.24456
H 1.63393 -1.28613 2.62184
H 2.07490 0.47158 2.77282
C 0.99803 1.97040 -1.15230
O 1.40747 2.79191 -1.90107
P -1.60755 1.98219 0.25431
H -0.00828 -0.74234 1.27343
H 0.92107 1.62786 1.15274
C -0.67866 -1.31148 0.53719
C -0.29721 -1.70385 -0.78053
C -1.24884 -2.25251 -1.68359
C -2.04579 -1.50501 0.89188
C -2.56262 -2.41031 -1.27191
C -2.98023 -2.05536 0.03220
H 0.76181 -1.80483 -1.01951
F 0.24439 -2.36902 1.93264
H -0.94367 -2.59712 -2.67496
F -2.43928 -1.14811 2.14517
F -3.48760 -2.94148 -2.11626
H -4.01218 -2.21211 0.35454
C -3.09532 1.61235 -0.81300
C -2.32665 2.02919 1.97525
C -1.37363 3.80602 -0.07026
H -2.81436 1.75673 -1.86841
H -3.38875 0.56087 -0.67232
H -3.94260 2.27367 -0.56505
H -1.55725 2.41981 2.65977
H -3.21516 2.68176 2.00861
H -2.59258 1.01138 2.29140
H -1.05875 3.96312 -1.11304
H -2.30793 4.35954 0.11936
H -0.57938 4.18472 0.59185

TS(2'-3')_1,2,4-C6F3H3_2

SCF (BP86) Energy = -1170.69789309
Enthalpy 0K = -1170.364580
Enthalpy 298K = -1170.336236
Free Energy 298K = -1170.424906
Imaginary Frequency = -574.5559 cm⁻¹
Ru 0.93922 -0.57331 0.11179
C -0.65015 -1.88605 0.22562
N -1.51301 -2.08979 1.28341
C -2.45392 -3.07646 0.99979
C -2.19634 -3.51047 -0.27123
N -1.10392 -2.77680 -0.72805
C -1.43651 -1.37390 2.55572
C -0.50321 -2.93132 -2.05372
H -2.69446 -4.25677 -0.88459
H -3.22140 -3.36984 1.71105
C 2.14126 -1.86706 -0.43951
O 2.91316 -2.69358 -0.79706

P 2.67499 1.01790 0.32902
C 4.30650 0.31301 0.90679
C 3.20443 1.97556 -1.18846
C 2.41163 2.37874 1.58103
H -0.29066 0.71321 0.48709
H 1.31088 -0.98328 1.57888
C -1.18013 1.28839 -0.56034
C -1.04777 2.70892 -0.48174
C -2.08972 3.53975 -0.09470
C -2.51283 0.78826 -0.46808
C -3.38300 3.01793 0.10641
C -3.55037 1.64253 -0.09337
F 0.20462 3.24024 -0.66292
F -0.36314 0.66018 -1.60440
H -1.88659 4.60873 0.01897
H -2.70910 -0.27497 -0.61547
H -4.22606 3.64929 0.39150
F -4.79417 1.10428 0.05535
H 0.43474 -3.50551 -1.99444
H -1.21570 -3.45818 -2.70598
H -0.29088 -1.93871 -2.47643
H -2.44176 -1.32142 3.00086
H -0.74939 -1.88526 3.25036
H -1.05574 -0.36078 2.36191
H 4.02799 2.67325 -0.96016
H 3.53220 1.26178 -1.96090
H 2.33642 2.53465 -1.56656
H 3.30986 3.01164 1.68056
H 1.55852 2.98969 1.25392
H 2.17310 1.92145 2.55412
H 5.07063 1.10093 1.01424
H 4.15276 -0.18689 1.87596
H 4.65221 -0.44058 0.18243

TS(5'-6')_1,2,4-C6F3H3_2

SCF (BP86) Energy = -1170.69848195
Enthalpy 0K = -1170.361822
Enthalpy 298K = -1170.334041
Free Energy 298K = -1170.419714
Imaginary Frequency = -380.9856 cm⁻¹
Ru 0.16329 0.71646 0.03208
C 2.18178 0.18221 0.22742
N 2.88195 -0.02440 1.39227
C 4.21678 -0.31178 1.13732
C 4.38214 -0.27654 -0.21946
N 3.13464 0.02021 -0.76091
C 2.28259 -0.06857 2.73422
C 2.90440 0.18407 -2.19676
H 3.56741 -0.50171 -2.74624
H 1.85806 -0.06224 -2.42420
H 3.10239 1.22057 -2.51406
H 5.26145 -0.43415 -0.83811
H 4.92120 -0.53019 1.93525
H 3.09678 -0.12120 3.47223
H 1.62180 -0.96155 2.78514
H 1.69831 0.85079 2.89757
C 0.60005 2.07140 -1.09862
O 0.89309 2.94561 -1.84189
P -2.04585 1.61464 0.14148
H -0.02461 -0.79849 1.33285
H 0.44529 1.74575 1.20131
C -0.56968 -1.43175 0.55122
C -0.04467 -1.72007 -0.74435
C -0.85567 -2.41364 -1.67368
C -1.89124 -1.88003 0.83174
C -2.14323 -2.84398 -1.38596
C -2.65440 -2.57832 -0.08846
H 1.02676 -1.66690 -0.93761

F 0.51205 -2.28790 2.01394
F -0.31084 -2.69786 -2.88831
F -2.41130 -1.61583 2.06520
H -2.72589 -3.39297 -2.12864
H -3.65709 -2.90945 0.19716
C -3.35060 0.98211 -1.03576
C -2.88821 1.51664 1.80250
C -2.12749 3.45240 -0.17811
H -3.02468 1.19724 -2.06596
H -3.44300 -0.10869 -0.92078
H -4.32606 1.46306 -0.85165
H -2.25969 2.04217 2.53872
H -3.88326 1.99073 1.76298
H -2.98069 0.46561 2.10804
H -1.76792 3.67200 -1.19483
H -3.15936 3.82340 -0.06448
H -1.46945 3.96613 0.54006

TS (2'-3')_1,2,4-C6F3H3_4

SCF (BP86) Energy = -1170.68855840
Enthalpy 0K = -1170.355647
Enthalpy 298K = -1170.327138
Free Energy 298K = -1170.416783
Imaginary Frequency = -521.7403 cm-1
Ru 1.20825 0.30664 0.08244
C 1.32792 -1.75396 0.21130
N 0.99212 -2.54917 1.28897
C 1.20922 -3.89865 1.02266
C 1.68535 -3.97497 -0.25664
N 1.75192 -2.66840 -0.73486
C 0.50033 -2.03572 2.56670
C 2.16562 -2.32609 -2.09423
H 1.97293 -4.83173 -0.86054
H 1.00823 -4.67549 1.75583
C 2.98109 0.53737 -0.40513
O 4.11895 0.69933 -0.69483
P 0.88167 2.62931 0.29147
C 2.34450 3.60378 0.92242
C 0.42532 3.61995 -1.23276
C -0.44322 3.14075 1.50631
H -0.56255 0.10169 0.44859
H 1.72568 0.37859 1.56312
C -1.54881 -0.18445 -0.56519
C -2.52733 0.85805 -0.60772
C -3.85512 0.58075 -0.29055
C -2.02155 -1.52678 -0.41046
C -4.28957 -0.72801 -0.02512
C -3.36274 -1.77407 -0.10004
H -2.24237 1.88565 -0.84064
F -0.50586 -0.02701 -1.62613
F -4.76069 1.59116 -0.27394
H -1.30918 -2.35249 -0.46806
F -5.59325 -0.96184 0.28203
H -3.71297 -2.79677 0.07044
H 3.16415 -2.74287 -2.30311
H 1.44113 -2.71676 -2.82755
H 2.20510 -1.23144 -2.17262
H -0.05351 -2.83450 3.08301
H 1.33740 -1.69674 3.19900
H -0.16375 -1.18132 2.37223
H 0.26686 4.68535 -0.99458
H 1.24072 3.52596 -1.96778
H -0.48859 3.20388 -1.68414
H -0.56206 4.23677 1.54308
H -1.39947 2.67320 1.22351
H -0.15901 2.76769 2.50285
H 2.10255 4.67426 1.02967
H 2.64671 3.19261 1.89820

H 3.18624 3.48237 0.22303

TS (5'-6')_1,2,4-C6F3H3_4

SCF (BP86) Energy = -1170.68921675
Enthalpy 0K = -1170.352757
Enthalpy 298K = -1170.324811
Free Energy 298K = -1170.411392
Imaginary Frequency = -335.0899 cm-1
Ru 0.52438 0.67161 0.02417
C 2.33208 -0.38750 0.04955
N 3.05953 -0.77347 1.15047
C 4.23920 -1.40792 0.78239
C 4.27801 -1.42073 -0.58425
N 3.10881 -0.80134 -1.01684
C 2.60329 -0.64776 2.54263
C 2.79003 -0.58888 -2.42845
H 3.18625 -1.43113 -3.01654
H 1.69810 -0.54209 -2.54448
H 3.22608 0.35364 -2.79698
H 5.02027 -1.80954 -1.27611
H 4.93305 -1.80507 1.51823
H 3.43205 -0.94429 3.20268
H 1.71675 -1.30743 2.67338
H 2.33455 0.40217 2.74009
C 1.20101 1.85646 -1.18159
O 1.64664 2.61933 -1.97086
P -1.33798 2.13416 0.30769
H 0.04700 -0.68886 1.36474
H 1.18298 1.58409 1.13994
C -0.72422 -1.18493 0.67309
C -0.40885 -1.63918 -0.64498
C -1.44646 -2.09448 -1.50416
C -2.08587 -1.20754 1.10325
C -2.76116 -2.10338 -1.06950
C -3.06578 -1.68774 0.25260
H 0.62087 -1.88045 -0.90904
F 0.20310 -2.26034 2.09050
H -1.21512 -2.49001 -2.49764
H -2.35291 -0.91558 2.12016
F -3.76989 -2.53878 -1.86486
F -4.35800 -1.73844 0.65582
C -2.82535 1.96083 -0.80936
C -2.11045 2.20746 2.00762
C -0.90501 3.93452 0.06539
H -2.49810 2.10330 -1.85151
H -3.23516 0.94481 -0.70842
H -3.60413 2.70237 -0.56410
H -1.32117 2.41980 2.74547
H -2.87731 2.99877 2.04983
H -2.57318 1.24122 2.25188
H -0.52722 4.09062 -0.95647
H -1.78283 4.57919 0.23593
H -0.10513 4.20295 0.77313

TS (2'-3')_1,3,5-C6F3H3_1

SCF (BP86) Energy = -1170.69831539
Enthalpy 0K = -1170.365410
Enthalpy 298K = -1170.336902
Free Energy 298K = -1170.426856
Imaginary Frequency = -541.2145 cm-1
Ru -1.20257 0.05130 0.08295
C -0.56506 2.01559 0.20309
N 0.06776 2.62800 1.26615
C 0.35508 3.96338 0.99645
C -0.09480 4.21417 -0.26992
N -0.64978 3.02515 -0.73738
C 0.37940 1.96277 2.53069
C -1.19722 2.86498 -2.08304

H	-0.06269	5.11847	-0.87203
H	0.85067	4.60829	1.71739
C	-2.94883	0.47829	-0.37005
O	-4.07460	0.73773	-0.63418
P	-1.72935	-2.23446	0.29230
C	-3.43920	-2.62488	0.93380
C	-1.66600	-3.31481	-1.23750
C	-0.66385	-3.18709	1.49549
H	0.51048	-0.40261	0.44179
H	-1.67945	0.16715	1.57303
C	1.54253	-0.48082	-0.59848
C	2.08255	-1.80525	-0.62129
C	3.41304	-1.99718	-0.25613
C	2.44881	0.61261	-0.42323
C	4.29865	-0.95368	0.04513
C	3.76531	0.33945	-0.06487
H	1.45681	-2.66285	-0.87141
F	0.52571	-0.25672	-1.64741
F	3.88571	-3.27275	-0.21781
H	2.09994	1.64387	-0.48683
H	5.33593	-1.13341	0.32672
F	4.59225	1.39435	0.17571
H	-1.98817	3.61102	-2.26275
H	-0.40225	2.98019	-2.83803
H	-1.62544	1.85660	-2.15896
H	1.17029	2.52944	3.04475
H	-0.51518	1.90807	3.17229
H	0.72614	0.94108	2.31908
H	-1.89494	-4.36820	-1.00334
H	-2.39952	-2.93313	-1.96569
H	-0.66661	-3.24797	-1.69453
H	-0.94179	-4.25394	1.53074
H	0.39346	-3.08725	1.20355
H	-0.78917	-2.74072	2.49454
H	-3.59420	-3.71162	1.03854
H	-3.56801	-2.13654	1.91233
H	-4.18739	-2.20895	0.24125

TS(5'-6')_1,3,5-C6F3H3_1

SCF (BP86) Energy =	-1170.69905453		
Enthalpy 0K =	-1170.362695		
Enthalpy 298K =	-1170.334780		
Free Energy 298K =	-1170.421147		
Imaginary Frequency =	-378.3783	cm-1	
Ru	0.33602	0.71470	0.05766
C	2.26709	-0.09076	0.18151
N	3.00925	-0.32418	1.31453
C	4.27011	-0.81643	1.00256
C	4.34611	-0.88855	-0.36066
N	3.11852	-0.44867	-0.84740
C	2.50085	-0.20230	2.68835
C	2.81822	-0.33805	-2.27532
H	3.33767	-1.14535	-2.81414
H	1.73451	-0.44025	-2.42415
H	3.14136	0.63721	-2.67381
H	5.15053	-1.20866	-1.01733
H	4.98959	-1.08514	1.77117
H	3.34516	-0.33915	3.38030
H	1.71854	-0.98006	2.83010
H	2.07263	0.80329	2.82549
C	0.89778	1.93731	-1.16650
O	1.26616	2.72605	-1.96982
P	-1.71905	1.91844	0.19408
H	-0.00587	-0.68930	1.45167
H	0.81930	1.74867	1.15796
C	-0.70110	-1.25480	0.73748
C	-0.27446	-1.66089	-0.56710
C	-1.23105	-2.24819	-1.42655

C	-2.05445	-1.46307	1.13069
C	-2.55704	-2.46162	-1.07196
C	-2.91989	-2.08169	0.24066
H	0.77933	-1.81242	-0.79966
F	0.39341	-2.15983	2.19603
F	-0.80692	-2.66098	-2.64941
H	-2.39201	-1.20143	2.13404
H	-3.26873	-2.94069	-1.74555
F	-4.20585	-2.29932	0.62016
C	-3.08509	1.50965	-1.01252
C	-2.60891	1.92454	1.83659
C	-1.51874	3.75476	-0.07920
H	-2.71528	1.69854	-2.03295
H	-3.33420	0.44128	-0.92529
H	-3.98532	2.11998	-0.82924
H	-1.90404	2.24202	2.62079
H	-3.46575	2.61811	1.80830
H	-2.96745	0.91232	2.06902
H	-1.09340	3.93718	-1.07770
H	-2.48604	4.27594	0.01023
H	-0.81571	4.14779	0.67189

TS(2'-3')_1,2-C6F2H4_1

SCF (BP86) Energy =	-1071.46400602		
Enthalpy 0K =	-1071.122674		
Enthalpy 298K =	-1071.095282		
Free Energy 298K =	-1071.181503		
Imaginary Frequency =	-572.4831	cm-1	
Ru	0.39821	-0.82947	0.10601
C	-1.62515	-1.21305	0.22734
N	-2.46655	-1.02960	1.30571
C	-3.76876	-1.43166	1.01881
C	-3.76669	-1.87406	-0.27542
N	-2.46217	-1.73078	-0.74210
C	-2.03751	-0.50082	2.59915
C	-2.02238	-2.08357	-2.09270
H	-4.56877	-2.26243	-0.89769
H	-4.57325	-1.35956	1.74594
C	0.81679	-2.52790	-0.49443
O	1.08446	-3.61438	-0.88860
P	2.69059	-0.28992	0.32408
C	3.76737	-1.71193	0.88292
C	3.62041	0.30264	-1.18732
C	3.13161	1.00828	1.59287
H	-0.06211	0.89127	0.50594
H	0.53690	-1.40655	1.55880
C	-0.54517	1.83265	-0.51598
C	0.26961	3.00159	-0.44488
C	-0.22215	4.24529	-0.07091
C	-1.95153	2.06372	-0.42587
C	-1.60608	4.42293	0.12062
C	-2.45653	3.32012	-0.06998
F	1.62179	2.84394	-0.62607
F	-0.14374	0.88087	-1.57756
H	0.48695	5.07258	0.03255
H	-2.62476	1.21634	-0.57952
H	-2.00389	5.40442	0.39158
H	-3.54057	3.44028	0.03331
H	-1.46671	-3.03448	-2.08758
H	-2.90716	-2.17865	-2.73994
H	-1.37120	-1.28741	-2.48175
H	-2.89212	-0.00987	3.08930
H	-1.65483	-1.30942	3.24401
H	-1.23123	0.22676	2.42755
H	4.68007	0.50642	-0.95763
H	3.55692	-0.47248	-1.96757
H	3.13549	1.21814	-1.55563
H	4.22505	1.11782	1.69151

H 2.68680 1.96336 1.27988
H 2.70161 0.71319 2.56291
H 4.82061 -1.40288 0.99033
H 3.39078 -2.08220 1.84931
H 3.69520 -2.53013 0.14977

TS(5'-6')_1,2-C6F2H4_1

SCF (BP86) Energy = -1071.46372198
Enthalpy 0K = -1071.118950
Enthalpy 298K = -1071.092112
Free Energy 298K = -1071.175475
Imaginary Frequency = -349.4915 cm-1

Ru -0.15294 0.62410 -0.09125
C -2.16954 0.05300 -0.15383
N -2.85951 -0.46552 -1.22385
C -4.19827 -0.66803 -0.91427
C -4.37755 -0.25891 0.37801
N -3.13376 0.17288 0.82980
C -2.24765 -0.87858 -2.49573
C -2.91526 0.72536 2.16625
H -3.57962 0.21345 2.87960
H -1.86849 0.55727 2.45585
H -3.11848 1.80829 2.18671
H -5.26395 -0.23747 1.00621
H -4.89572 -1.09676 -1.62867
H -3.05544 -1.13958 -3.19561
H -1.58409 -1.74734 -2.28805
H -1.66518 -0.03787 -2.90468
C -0.61004 2.24512 0.59489
O -0.92263 3.29516 1.04564
P 2.06913 1.44637 -0.38580
H 0.03844 -1.16121 -0.92007
H -0.40555 1.27485 -1.51001
C 0.57209 -1.59985 -0.00585
C 0.07099 -1.55577 1.32925
C 0.87801 -1.99235 2.41301
C 1.88750 -2.11377 -0.18156
C 2.16275 -2.48604 2.19601
C 2.66635 -2.56237 0.87098
H -0.99609 -1.39539 1.49277
F -0.51122 -2.80911 -1.17139
H 0.45566 -1.98443 3.42337
F 2.38501 -2.17453 -1.45092
H 2.77649 -2.84026 3.02942
H 3.66005 -2.96833 0.65872
C 3.32902 1.13018 0.95550
C 2.95481 0.91022 -1.93747
C 2.17436 3.30299 -0.55708
H 2.97749 1.60958 1.88303
H 3.40274 0.04594 1.13094
H 4.31795 1.53639 0.68377
H 2.35842 1.23743 -2.80385
H 3.95863 1.36421 -1.98938
H 3.03167 -0.18527 -1.96059
H 1.79222 3.78543 0.35530
H 3.21512 3.62103 -0.73336
H 1.54450 3.61696 -1.40412

TS(2'-3')_1,3-C6F2H4_1

SCF (BP86) Energy = -1071.46392685
Enthalpy 0K = -1071.123076
Enthalpy 298K = -1071.095491
Free Energy 298K = -1071.183510
Imaginary Frequency = -527.5641 cm-1

Ru 0.75912 0.69200 0.07657
C 1.81655 -1.07995 0.21085
N 1.88979 -1.93285 1.29398
C 2.70489 -3.03104 1.03244

C 3.15897 -2.88706 -0.24905
N 2.61216 -1.70114 -0.73364
C 1.21543 -1.69846 2.57006
C 2.82140 -1.21256 -2.09505
H 3.80813 -3.51792 -0.85071
H 2.88644 -3.80881 1.76966
C 2.22282 1.70852 -0.43191
O 3.15595 2.37396 -0.73452
P -0.59734 2.60593 0.28393
C 0.25895 4.14858 0.89637
C -1.46980 3.26304 -1.23892
C -1.99812 2.45771 1.51149
H -0.71235 -0.29323 0.47047
H 1.19749 1.00264 1.55228
C -1.46883 -1.00361 -0.54273
C -2.81306 -0.51976 -0.56992
C -3.85170 -1.37990 -0.21741
C -1.27152 -2.41156 -0.36736
C -3.66546 -2.73679 0.07464
C -2.35001 -3.23034 -0.02571
H -3.03113 0.52040 -0.81799
F -0.62166 -0.39725 -1.61224
F -5.11569 -0.86988 -0.19221
H -0.26020 -2.81823 -0.43874
H -4.51459 -3.37040 0.33721
H -2.16471 -4.29569 0.15226
H 3.89754 -1.07567 -2.28985
H 2.40063 -1.92204 -2.82629
H 2.30921 -0.24610 -2.19224
H 1.12310 -2.65583 3.10500
H 1.78485 -0.98302 3.18576
H 0.21820 -1.27956 2.37293
H -2.10269 4.13520 -1.00288
H -0.70784 3.55258 -1.98028
H -2.08891 2.46711 -1.68078
H -2.60835 3.37589 1.54716
H -2.63266 1.59976 1.23870
H -1.56512 2.26430 2.50553
H -0.44701 4.98904 1.00260
H 0.72361 3.92970 1.87041
H 1.05710 4.42214 0.18887

TS(5'-6')_1,3-C6F2H4_1

SCF (BP86) Energy = -1071.46323177
Enthalpy 0K = -1071.118878
Enthalpy 298K = -1071.091853
Free Energy 298K = -1071.176329
Imaginary frequency = -351.4280 cm-1

Ru 0.29851 0.62479 0.08686
C 2.24028 -0.16449 0.10016
N 2.95034 -0.62623 1.18278
C 4.23214 -1.01852 0.81916
C 4.35537 -0.79187 -0.52352
N 3.13426 -0.27636 -0.94870
C 2.39533 -0.81244 2.53137
C 2.87704 0.13638 -2.32787
H 3.41284 -0.54004 -3.01186
H 1.79732 0.07508 -2.52306
H 3.20977 1.17273 -2.50088
H 5.18859 -0.94905 -1.20309
H 4.93185 -1.43601 1.53800
H 3.21948 -1.08777 3.20628
H 1.62356 -1.61193 2.47035
H 1.94472 0.13436 2.86897
C 0.87843 2.09829 -0.81058
O 1.26473 3.05092 -1.39973
P -1.79128 1.72748 0.40582
H -0.04165 -1.02963 1.12161

H	0.72031	1.39016	1.40682
C	-0.70918	-1.47322	0.29996
C	-0.27988	-1.61162	-1.05712
C	-1.20867	-2.02893	-2.04515
C	-2.06021	-1.78154	0.63311
C	-2.53210	-2.32590	-1.72271
C	-2.91408	-2.22253	-0.36614
H	0.78482	-1.63263	-1.29364
F	0.36771	-2.64811	1.54854
H	-0.86137	-2.16859	-3.07481
H	-2.40337	-1.73514	1.66785
H	-3.25392	-2.67258	-2.46603
F	-4.19516	-2.54246	-0.03752
C	-3.11185	1.54480	-0.90255
C	-2.72502	1.37275	1.98450
C	-1.64016	3.58530	0.52342
H	-2.72139	1.95144	-1.84907
H	-3.32914	0.47563	-1.04690
H	-4.03485	2.08130	-0.62525
H	-2.05322	1.54456	2.83992
H	-3.60487	2.03222	2.06837
H	-3.05354	0.32435	1.99490
H	-1.19484	3.98048	-0.40221
H	-2.62484	4.05316	0.68739
H	-0.96921	3.83225	1.36112

TS (2'-3')_1,4-C6F2H4_1

SCF (BP86) Energy =	-1071.46013501		
Enthalpy 0K =	-1071.119292		
Enthalpy 298K =	-1071.091730		
Free Energy 298K =	-1071.179253		
Imaginary Frequency =	-507.8707	cm-1	
Ru	-1.09233	0.00079	0.08230
C	-0.50437	1.97825	0.22482
N	0.08117	2.60631	1.30621
C	0.33630	3.95057	1.04702
C	-0.08460	4.19083	-0.23134
N	-0.59152	2.98738	-0.71609
C	0.36757	1.95004	2.58093
C	-1.09385	2.81200	-2.07728
H	-0.06284	5.09734	-0.83068
H	0.78930	4.60886	1.78382
C	-2.83944	0.38812	-0.39694
O	-3.96653	0.62223	-0.68062
P	-1.56965	-2.29563	0.27282
C	-3.26795	-2.72552	0.92038
C	-1.49361	-3.36397	-1.26509
C	-0.48057	-3.23831	1.46413
H	0.64914	-0.41621	0.43399
H	-1.60069	0.09776	1.56595
C	1.66250	-0.46985	-0.56940
C	2.23759	-1.77802	-0.63610
C	3.59324	-1.98262	-0.35389
C	2.56069	0.63418	-0.41771
C	4.42098	-0.88524	-0.09105
C	3.91420	0.42011	-0.13909
H	1.59620	-2.63041	-0.87458
F	0.61168	-0.25015	-1.63200
H	4.01819	-2.99079	-0.36569
H	2.16381	1.65144	-0.46112
F	5.74237	-1.08607	0.18738
H	4.58930	1.26646	0.02054
H	-1.88427	3.55056	-2.28754
H	-0.27636	2.92684	-2.80789
H	-1.51113	1.79942	-2.15804
H	1.17537	2.49660	3.09105
H	-0.52989	1.93230	3.22118
H	0.67964	0.91478	2.38189

H	-1.69832	-4.42398	-1.03812
H	-2.24027	-2.99220	-1.98501
H	-0.49922	-3.27017	-1.72825
H	-0.73605	-4.31115	1.49032
H	0.57380	-3.11366	1.17082
H	-0.61235	-2.80411	2.46771
H	-3.40198	-3.81592	1.01612
H	-3.40048	-2.24797	1.90372
H	-4.02746	-2.31741	0.23550

TS (5'-6')_1,4-C6F2H4_1

SCF (BP86) Energy =	-1071.46075301		
Enthalpy 0K =	-1071.116255		
Enthalpy 298K =	-1071.089302		
Free Energy 298K =	-1071.173415		
Imaginary Frequency =	-310.7252 cm-1		
Ru	0.25972	0.65691	0.00618
C	2.21074	-0.10490	0.01357
N	3.01522	-0.32722	1.10638
C	4.27189	-0.78246	0.72755
C	4.28039	-0.84555	-0.63824
N	3.01814	-0.43600	-1.05891
C	2.57856	-0.21019	2.50566
C	2.63327	-0.34212	-2.46688
H	3.15629	-1.12732	-3.03437
H	1.54745	-0.49073	-2.55043
H	2.88892	0.64507	-2.88435
H	5.05825	-1.14180	-1.33679
H	5.03696	-1.03422	1.45686
H	3.45589	-0.36434	3.15149
H	1.79534	-0.97952	2.68922
H	2.17271	0.80017	2.67339
C	0.69504	1.86394	-1.28754
O	0.98287	2.64387	-2.13189
P	-1.79647	1.82461	0.30593
H	0.02577	-0.66328	1.42065
H	0.80674	1.71949	1.04767
C	-0.66189	-1.33247	0.78351
C	-0.29913	-1.81587	-0.51157
C	-1.26613	-2.47046	-1.32291
C	-1.99876	-1.55076	1.24359
C	-2.55556	-2.64473	-0.84472
C	-2.92560	-2.21615	0.45052
H	0.75149	-1.90382	-0.79025
F	0.40879	-2.16899	2.24291
H	-0.98832	-2.88502	-2.29634
H	-2.26288	-1.24336	2.25796
F	-3.48773	-3.27563	-1.61251
H	-3.94014	-2.41531	0.80894
C	-3.28110	1.36120	-0.72823
C	-2.49999	1.86110	2.03717
C	-1.66558	3.65614	-0.03489
H	-3.02500	1.50205	-1.79035
H	-3.51138	0.29783	-0.56181
H	-4.15912	1.97977	-0.47672
H	-1.72856	2.24357	2.72351
H	-3.38848	2.51294	2.08058
H	-2.77850	0.84498	2.34978
H	-1.36036	3.81708	-1.08001
H	-2.62684	4.16324	0.15006
H	-0.88961	4.08235	0.62010

TS (2'-3')_C6FH5

SCF (BP86) Energy =	-972.228704945
Enthalpy 0K =	-971.879872
Enthalpy 298K =	-971.854111
Free Energy 298K =	-971.936497
Imaginary Frequency =	-503.1849 cm-1

Ru	0.44654	-0.73806	0.07557
C	-1.57037	-1.16898	0.22301
N	-2.39646	-0.96087	1.30945
C	-3.69990	-1.37941	1.05496
C	-3.71566	-1.85878	-0.22531
N	-2.41903	-1.72449	-0.71614
C	-1.95150	-0.39492	2.58195
C	-2.03016	-2.08020	-2.07920
H	-4.52485	-2.27113	-0.82246
H	-4.49139	-1.29855	1.79549
C	0.93771	-2.45263	-0.42533
O	1.26856	-3.55160	-0.72311
P	2.69343	-0.06540	0.27187
C	3.87677	-1.36037	0.91336
C	3.60261	0.52067	-1.25856
C	2.99926	1.33152	1.47516
H	-0.01270	0.98218	0.45250
H	0.60780	-1.24612	1.55436
C	-0.44805	1.90503	-0.55096
C	0.43371	3.02993	-0.60137
C	-0.03426	4.31042	-0.28806
C	-1.84478	2.16838	-0.38681
C	-1.39163	4.54457	-0.00418
C	-2.28476	3.45853	-0.07805
H	1.48586	2.86971	-0.85230
F	-0.14491	0.88509	-1.62094
H	0.67683	5.14481	-0.29459
H	-2.55125	1.33621	-0.44533
H	-1.74981	5.55030	0.23295
H	-3.35658	3.62038	0.08736
H	-2.25340	-3.14173	-2.27444
H	-2.56515	-1.44945	-2.80793
H	-0.94973	-1.91158	-2.17929
H	-2.82132	0.02616	3.10873
H	-1.47733	-1.16854	3.20816
H	-1.21498	0.39565	2.37888
H	4.63335	0.83801	-1.02619
H	3.62855	-0.30604	-1.98648
H	3.05200	1.35802	-1.71434
H	4.06362	1.61994	1.50523
H	2.38512	2.19964	1.18757
H	2.67958	0.99912	2.47537
H	4.89932	-0.96054	1.01658
H	3.51551	-1.71203	1.89232
H	3.88180	-2.21694	0.22143

TS (5'-6')_C6FH5

SCF (BP86) Energy =	-972.228278613
Enthalpy 0K =	-971.875659
Enthalpy 298K =	-971.849667
Free Energy 298K =	-971.931211
Imaginary Frequency =	-323.2021 cm ⁻¹

Ru	-0.02050	-0.54086	0.08833
C	-2.08420	-0.17783	0.10691
N	-2.86798	0.14383	1.18965
C	-4.20610	0.25286	0.83328
C	-4.28801	-0.01612	-0.50479
N	-2.98889	-0.27153	-0.93461
C	-2.35490	0.45648	2.53162
C	-2.65781	-0.63591	-2.31165
H	-3.34511	-0.11469	-2.99595
H	-1.62484	-0.32665	-2.52401
H	-2.74057	-1.72395	-2.46598
H	-5.14004	-0.04691	-1.17851
H	-4.97300	0.52572	1.55303
H	-3.21512	0.58089	3.20631
H	-1.75046	1.38858	2.45651
H	-1.73092	-0.38082	2.88259

C	-0.27409	-2.10453	-0.81083
O	-0.44811	-3.11831	-1.39941
P	2.25373	-1.17523	0.41101
H	-0.01582	1.13263	1.11471
H	-0.27132	-1.37476	1.41138
C	0.52244	1.71730	0.28227
C	0.04523	1.76964	-1.06337
C	0.85421	2.35673	-2.07210
C	1.78969	2.30423	0.58223
C	2.09874	2.90632	-1.76878
C	2.54470	2.90143	-0.42146
H	-1.00561	1.57079	-1.28042
F	-0.70809	2.66100	1.57140
H	0.46059	2.42037	-3.09304
H	2.12545	2.32518	1.62200
H	2.70802	3.37193	-2.54968
H	3.50135	3.37141	-0.16560
C	3.50979	-0.71345	-0.89118
C	3.08328	-0.62905	1.99364
C	2.50109	-3.02272	0.53094
H	3.21459	-1.18626	-1.84143
H	3.49589	0.37925	-1.02500
H	4.52378	-1.04778	-0.61369
H	2.46452	-0.94898	2.84647
H	4.08777	-1.07637	2.07812
H	3.16846	0.46634	2.00785
H	2.15632	-3.50357	-0.39708
H	3.56162	-3.27055	0.70215
H	1.89202	-3.40662	1.36436

Fluoroarenes

C6F6

SCF (BP86) Energy =	-827.594693280
Enthalpy 0K =	-827.544838
Enthalpy 298K =	-827.534795
Free Energy 298K =	-827.580356

C	1.21603	-0.70207	0.00000
C	0.00002	-1.40420	0.00000
C	-1.21602	-0.70210	0.00000
C	-1.21603	0.70205	0.00000
C	-0.00002	1.40417	0.00000
C	1.21601	0.70208	0.00000
F	2.38028	-1.37420	0.00000
F	0.00004	-2.74840	0.00000
F	-2.38025	-1.37427	0.00000
F	-2.38029	1.37417	0.00000
F	-0.00004	2.74851	0.00000
F	2.38026	1.37424	0.00000

C6F5H

SCF (BP86) Energy =	-728.377917923
Enthalpy 0K =	-728.320057
Enthalpy 298K =	-728.311085
Free Energy 298K =	-728.354247

C	-1.20416	-0.97607	0.00000
C	-0.00000	-1.68768	0.00000
C	1.20416	-0.97607	0.00000
C	1.21900	0.42795	0.00000
C	0.00000	1.12564	0.00000
C	-1.21899	0.42795	0.00000
F	-2.38143	-1.63401	-0.00000
H	0.00000	-2.77964	0.00000
F	2.38142	-1.63402	-0.00000
F	2.38114	1.10635	0.00000
F	0.00001	2.46971	0.00000
F	-2.38114	1.10635	0.00000

1,2,3,4-C6F4H2

SCF (BP86) Energy = -629.154259470
Enthalpy 0K = -629.088389
Enthalpy 298K = -629.080379
Free Energy 298K = -629.121290
C 0.70266 -1.74514 0.00000
C -0.70243 -1.74518 0.00000
C -1.39486 -0.53180 0.00000
C -0.70147 0.69137 0.00000
C 0.70141 0.69144 0.00000
C 1.39497 -0.53160 0.00000
H 1.26986 -2.67887 0.00000
H -1.26937 -2.67892 0.00000
F -2.74535 -0.50387 0.00000
F -1.37139 1.85830 0.00000
F 1.37112 1.85854 0.00000
F 2.74538 -0.50372 0.00000

1,2,3,5-C6F4H2

SCF (BP86) Energy = -629.160051764
Enthalpy 0K = -629.094180
Enthalpy 298K = -629.086236
Free Energy 298K = -629.127053
C 0.38582 -1.20735 0.00000
C -1.01291 -1.22836 0.00000
C -1.68463 -0.00013 0.00000
C -1.01309 1.22818 0.00000
C 0.38571 1.20745 0.00000
C 1.10311 0.00011 0.00000
F 1.07883 -2.36421 0.00000
H -1.55529 -2.17517 0.00000
F -3.03781 -0.00019 0.00000
H -1.55577 2.17492 0.00000
F 1.07838 2.36443 0.00000
F 2.45027 0.00007 0.00000

1,2,4,5-C6F4H2

SCF (BP86) Energy = -629.159485237
Enthalpy 0K = -629.093656
Enthalpy 298K = -629.085712
Free Energy 298K = -629.126540
C -1.20619 -0.70253 0.00000
C 0.00000 -1.41085 0.00000
C 1.20619 -0.70253 0.00000
C 1.20618 0.70253 0.00000
C 0.00000 1.41089 0.00000
C -1.20618 0.70254 0.00000
F -2.38284 -1.36442 0.00000
H 0.00000 -2.50275 0.00000
F 2.38284 -1.36442 0.00000
F 2.38283 1.36443 0.00000
H 0.00000 2.50231 0.00000
F -2.38283 1.36443 0.00000

1,2,3-C6F3H3

SCF (BP86) Energy = -529.929593921
Enthalpy 0K = -529.855709
Enthalpy 298K = -529.848638
Free Energy 298K = -529.887305
C 1.22131 1.38465 0.00000
C 0.00000 2.07735 0.00000
C -1.22131 1.38465 0.00000
C -1.20922 -0.01418 0.00000
C 0.00000 -0.72828 0.00000
C 1.20922 -0.01418 0.00000
H 2.18227 1.90477 0.00000
H 0.00000 3.17085 0.00000
H -2.18227 1.90477 0.00000
F -2.36510 -0.71336 0.00000

F 0.00000 -2.07556 0.00000
F 2.36510 -0.71336 0.00000

1,2,4-C6F3H3

SCF (BP86) Energy = -529.934782581
Enthalpy 0K = -529.860944
Enthalpy 298K = -529.853931
Free Energy 298K = -529.892527
C -1.20660 -1.05357 0.00000
C 0.01266 -1.75143 0.00000
C 1.20572 -1.02059 0.00000
C 1.22376 0.38078 0.00000
C 0.00000 1.05503 0.00000
C -1.21320 0.34358 0.00000
H -2.16227 -1.58443 0.00000
H 0.04279 -2.84326 0.00000
F 2.38861 -1.68247 0.00000
H 2.16383 0.93624 0.00000
F -0.02997 2.40474 0.00000
F -2.37847 1.02981 0.00000

1,3,5-C6F3H3

SCF (BP86) Energy = -529.941612251
Enthalpy 0K = -529.867755
Enthalpy 298K = -529.860808
Free Energy 298K = -529.899310
C 1.19887 -0.68094 0.00000
C 0.01002 -1.42023 0.00000
C -1.18914 -0.69779 0.00000
C -1.23490 0.70139 0.00000
C -0.00973 1.37875 0.00000
C 1.22487 0.71876 0.00000
F 2.37553 -1.34924 0.00000
H 0.01772 -2.51109 0.00000
F -2.35625 -1.38264 0.00000
H -2.18391 1.24035 0.00000
F -0.01928 2.73188 0.00000
H 2.16618 1.27105 0.00000

1,2-C6F2H4

SCF (BP86) Energy = -430.703359171
Enthalpy 0K = -430.621516
Enthalpy 298K = -430.615352
Free Energy 298K = -430.651792
C -0.32975 -1.52379 0.00000
C 1.06448 -1.70148 0.00000
C 1.91904 -0.58772 0.00000
C 1.38648 0.71298 0.00000
C 0.00000 0.88597 0.00000
C -0.85577 -0.22936 0.00000
H -1.02022 -2.37197 0.00000
H 1.47806 -2.71426 0.00000
H 3.00451 -0.72504 0.00000
H 2.02701 1.59948 0.00000
F -0.53940 2.12635 0.00000
F -2.19351 -0.02945 0.00000

1,3-C6F2H4

SCF (BP86) Energy = -430.709488427
Enthalpy 0K = -430.627645
Enthalpy 298K = -430.621537
Free Energy 298K = -430.657911
C 1.22304 1.09163 0.00000
C 0.00000 1.78118 0.00000
C -1.22304 1.09163 0.00000
C -1.19541 -0.30851 0.00000
C 0.00000 -1.03665 0.00000
C 1.19541 -0.30851 0.00000

H	2.18193	1.61492	0.00000
H	0.00000	2.87551	0.00000
H	-2.18193	1.61492	0.00000
F	-2.36648	-0.99120	0.00000
H	0.00000	-2.12834	0.00000
F	2.36648	-0.99120	0.00000

1,4-C6F2H4

SCF (BP86) Energy =	-430.708292243		
Enthalpy 0K =	-430.626507		
Enthalpy 298K =	-430.620385		
Free Energy 298K =	-430.656773		
C	0.91824	1.07140	0.00000
C	1.38864	-0.25060	0.00000
C	0.46303	-1.30135	0.00000
C	-0.91824	-1.07140	0.00000
C	-1.38862	0.25059	0.00000
C	-0.46303	1.30134	0.00000
H	1.60820	1.91956	0.00000
H	2.45901	-0.47227	0.00000
F	0.91824	-2.58070	0.00000
H	-1.60816	-1.91956	0.00000
H	-2.45922	0.47233	0.00000
F	-0.91824	2.58070	0.00000

C6FH5

SCF (BP86) Energy =	-331.476231929		
Enthalpy 0K =	-331.386447		
Enthalpy 298K =	-331.381147		
Free Energy 298K =	-331.415373		
C	-0.93837	-0.00002	0.00000
C	-0.26152	-1.22526	0.00000
C	1.14249	-1.21556	0.00000
C	1.84708	0.00002	0.00000
C	1.14247	1.21559	0.00000
C	-0.26153	1.22523	0.00000
F	-2.29683	-0.00001	0.00000
H	-0.83289	-2.15748	0.00000
H	1.68606	-2.16630	0.00000
H	2.94157	0.00003	0.00000
H	1.68601	2.16628	0.00000
H	-0.83308	2.15761	0.00000

C6H6

SCF (BP86) Energy =	-232.242069561		
Enthalpy 0K =	-232.144358		
Enthalpy 298K =	-232.139827		
Free Energy 298K =	-232.171900		
C	-0.70236	1.21651	0.00000
C	-1.40487	0.00000	0.00000
C	-0.70236	-1.21651	0.00000
C	0.70239	-1.21655	0.00000
C	1.40480	0.00000	0.00000
C	0.70239	1.21655	0.00000
H	-1.24998	2.16513	0.00000
H	-2.50020	-0.00000	0.00000
H	-1.24998	-2.16513	0.00000
H	1.25002	-2.16515	0.00000
H	2.50013	0.00000	0.00000
H	1.25002	2.16515	0.00000

Radicals

[2,3-C6F2H3]•

SCF (BP86) Energy =	-430.012513354
Enthalpy 0K =	-429.943323
Enthalpy 298K =	-429.937143
Free Energy 298K =	-429.974271
C	0.34667 -1.50707 0.00000

C	0.90272	-0.24284	0.00000
C	0.00000	0.84323	0.00000
C	-1.38300	0.62403	0.00000
C	-1.88614	-0.68742	0.00000
C	-1.00576	-1.79370	0.00000
F	2.23343	-0.01653	0.00000
F	0.49484	2.10167	0.00000
H	-2.04830	1.49104	0.00000
H	-2.96796	-0.85473	0.00000
H	-1.38522	-2.81993	0.00000

[2,4-C6F2H3]•

SCF (BP86) Energy =	-430.016717437		
Enthalpy 0K =	-429.947553		
Enthalpy 298K =	-429.941443		
Free Energy 298K =	-429.978465		
C	-1.24996	-1.04039	0.00000
C	-1.23815	0.34564	0.00000
C	0.00000	1.00916	0.00000
C	1.16337	0.22564	0.00000
C	1.14077	-1.17553	0.00000
C	-0.11349	-1.82652	0.00000
F	-2.38185	1.06601	0.00000
H	0.05431	2.10147	0.00000
F	2.36176	0.85939	0.00000
H	2.07909	-1.73729	0.00000
H	-0.16780	-2.92077	0.00000

[2,5-C6F2H3]•

SCF (BP86) Energy =	-430.017057640		
Enthalpy 0K =	-429.947949		
Enthalpy 298K =	-429.941821		
Free Energy 298K =	-429.978870		
C	-0.00558	-1.39236	0.000000
C	1.21923	-0.74550	0.000000
C	1.21856	0.66042	0.000000
C	0.00000	1.35850	0.000000
C	-1.20622	0.64524	0.000000
C	-1.23516	-0.76509	0.000000
F	2.38926	-1.42599	0.000000
H	2.17563	1.19361	0.000000
H	-0.02305	2.45135	0.000000
F	-2.37901	1.32477	0.000000
H	-2.18975	-1.30116	0.000000

[2,6-C6F2H3]•

SCF (BP86) Energy =	-430.014037954		
Enthalpy 0K =	-429.944739		
Enthalpy 298K =	-429.938600		
Free Energy 298K =	-429.975720		
C	0.00000	1.01216	0.00000
C	1.21770	0.35480	0.00000
C	1.22619	-1.05242	0.00000
C	0.00000	-1.73766	0.00000
C	-1.22619	-1.05242	0.00000
C	-1.21770	0.35480	0.00000
F	2.38334	1.03964	0.00000
H	2.18504	-1.57885	0.00000
H	0.00000	-2.83128	0.00000
H	-2.18504	-1.57885	0.00000
F	-2.38334	1.03964	0.00000

[3,4-C6F2H3]•

SCF (BP86) Energy =	-430.014437264
Enthalpy 0K =	-429.945373
Enthalpy 298K =	-429.939218
Free Energy 298K =	-429.976252
C 1.12770 -1.65134 0.00000	

C -0.25685 -1.59947 0.00000
C -0.82387 -0.31367 0.00000
C 0.00000 0.82900 0.00000
C 1.39355 0.71382 0.00000
C 1.98927 -0.56817 0.00000
H -0.90431 -2.48207 0.00000
F -2.16501 -0.15185 0.00000
F -0.58513 2.04860 0.00000
H 1.99847 1.62641 0.00000
H 3.07835 -0.67620 0.00000

[3,5-C6F2H3]•

SCF (BP86) Energy = -430.021585073
Enthalpy 0K = -429.952526
Enthalpy 298K = -429.946420
Free Energy 298K = -429.983412
C 1.76826 0.00000 0.00000
C 1.15628 -1.24029 0.00000
C -0.25236 -1.20159 0.00000
C -0.97310 0.00000 0.00000
C -0.25236 1.20159 0.00000
C 1.15628 1.24029 0.00000
H 1.69099 -2.19418 0.00000
F -0.94086 -2.36825 0.00000
H -2.06455 0.00000 0.00000
F -0.94086 2.36825 0.00000
H 1.69099 2.19418 0.00000

[2,3,4-C6F3H2]•

SCF (BP86) Energy = -529.237405377
Enthalpy 0K = -529.176169
Enthalpy 298K = -529.169080
Free Energy 298K = -529.208443
C 1.27106 -1.31434 0.00000
C 1.25928 0.06858 0.00000
C 0.00000 0.70191 0.00000
C -1.16636 -0.08676 0.00000
C -1.10874 -1.48475 0.00000
C 0.15178 -2.12405 0.00000
F 2.37966 0.81848 0.00000
F -0.08998 2.04577 0.00000
F -2.35882 0.54786 0.00000
H -2.04151 -2.05675 0.00000
H 0.22159 -3.21586 0.00000

[2,3,5-C6F3H2]•

SCF (BP86) Energy = -529.243383383
Enthalpy 0K = -529.182166
Enthalpy 298K = -529.175123
Free Energy 298K = -529.214449
C 1.21995 -0.99999 0.00000
C 1.25368 0.38026 0.00000
C 0.00000 1.03109 0.00000
C -1.19557 0.30313 0.00000
C -1.13382 -1.09730 0.00000
C 0.09048 -1.79508 0.00000
F 2.39477 1.10046 0.00000
F -0.03331 2.38101 0.00000
H -2.15547 0.82267 0.00000
F -2.29103 -1.80001 0.00000
H 0.11324 -2.88846 0.00000

[2,3,6-C6F3H2]•

SCF (BP86) Energy = -529.239607455
Enthalpy 0K = -529.178269
Enthalpy 298K = -529.171207
Free Energy 298K = -529.210605
C 1.19113 0.39505 0.00000

C 0.00000 1.09228 0.00000
C -1.19147 0.33079 0.00000
C -1.13926 -1.06715 0.00000
C 0.09762 -1.73408 0.00000
C 1.28785 -0.98650 0.00000
F -0.05979 2.43858 0.00000
F -2.37721 0.97893 0.00000
H -2.07870 -1.62649 0.00000
H 0.15395 -2.82672 0.00000
F 2.48695 -1.60964 0.00000

[C6F3H2]•

SCF (BP86) Energy = -529.242100720
Enthalpy 0K = -529.180916
Enthalpy 298K = -529.173887
Free Energy 298K = -529.213167
C 0.00604 -1.73115 0.00000
C 1.22619 -1.07723 0.00000
C 1.22635 0.32923 0.00000
C 0.00000 1.00350 0.00000
C -1.22122 0.30255 0.00000
C -1.22591 -1.10397 0.00000
F 2.39927 -1.74802 0.00000
H 2.16437 0.89108 0.00000
F -0.02605 2.35333 0.00000
F -2.37938 0.99639 0.00000
H -2.17761 -1.64398 0.00000

[2,4,6-C6F3H2]•

SCF (BP86) Energy = -529.244715189
Enthalpy 0K = -529.183366
Enthalpy 298K = -529.176380
Free Energy 298K = -529.215659
C 0.00000 -1.39590 0.00000
C -1.21648 -0.73500 0.00000
C -1.23437 0.67071 0.00000
C 0.00000 1.33516 0.00000
C 1.23437 0.67071 0.00000
C 1.21648 -0.73500 0.00000
F -2.38121 -1.41680 0.00000
H -2.17784 1.22208 0.00000
F 0.00000 2.68825 0.00000
H 2.17783 1.22208 0.00000
F 2.38121 -1.41680 0.00000

[3,4,5-C6F3H2]•

SCF (BP86) Energy = -529.240526438
Enthalpy 0K = -529.179416
Enthalpy 298K = -529.172339
Free Energy 298K = -529.211638
C -0.00001 -2.06041 0.00000
C -1.23976 -1.44647 0.00000
C -1.21608 -0.03959 0.00000
C 0.00000 0.66674 0.00000
C 1.21608 -0.03959 0.00000
C 1.23975 -1.44648 0.00000
H -2.19373 -1.98050 0.00000
F -2.36533 0.66819 0.00000
F 0.00000 2.01428 0.00000
F 2.36533 0.66818 0.00000
H 2.19379 -1.98055 0.00000

[2,3,4,5-C6F4H]•

SCF (BP86) Energy = -628.461850111
Enthalpy 0K = -628.408611
Enthalpy 298K = -628.400556
Free Energy 298K = -628.442227
C 0.78149 -1.68070 0.00000

C -0.57685 -1.43271 0.00000
C -0.97203 -0.07797 0.00000
C 0.00000 0.93780 0.00000
C 1.36846 0.61101 0.00000
C 1.78612 -0.73214 0.00000
F -1.51361 -2.40186 0.00000
F -2.27658 0.25276 0.00000
F -0.38845 2.22629 0.00000
F 2.27028 1.61434 0.00000
H 2.85213 -0.97548 0.00000

[2,3,4,6-C6F4H]•

SCF (BP86) Energy = -628.463702356
Enthalpy 0K = -628.410330
Enthalpy 298K = -628.402315
Free Energy 298K = -628.443990
C 1.16491 -1.07459 0.00000
C -0.07892 -1.72954 0.00000
C -1.23142 -0.96372 0.00000
C -1.24216 0.41834 0.00000
C 0.00000 1.08743 0.00000
C 1.18262 0.32562 0.00000
H 2.09900 -1.64167 0.00000
F -0.12847 -3.07798 0.00000
F -2.38043 1.13677 0.00000
F 0.05169 2.43272 0.00000
F 2.36064 0.98188 0.00000

[2,3,5,6-C6F4H]•

SCF (BP86) Energy = -628.464091985
Enthalpy 0K = -628.410715
Enthalpy 298K = -628.402669
Free Energy 298K = -628.444433
C 1.36914 0.00000 0.00000
C 0.66569 1.21057 0.00000
C -0.74636 1.22900 0.00000
C -1.37689 0.00000 0.00000
C -0.74636 -1.22900 0.00000
C 0.66569 -1.21057 0.00000
H 2.46060 -0.00000 0.00000
F 1.33374 2.38352 0.00000
F -1.41409 2.39903 0.00000
F -1.41409 -2.39903 0.00000
F 1.33375 -2.38352 0.00000

[C6F5]•

SCF (BP86) Energy = -727.681718141
Enthalpy 0K = -727.636356
Enthalpy 298K = -727.627238
Free Energy 298K = -727.671446
C 0.00000 -1.65216 0.00000
C -1.22750 -1.01893 0.00000
C -1.22416 0.39160 0.00000
C 0.00000 1.08403 0.00000
C 1.22417 0.39160 0.00000
C 1.22750 -1.01892 0.00000
F -2.39776 -1.68450 0.00000
F -2.38135 1.07802 0.00000
F -0.00001 2.42814 0.00000
F 2.38135 1.07803 0.00000
F 2.39776 -1.68450 0.00000

[2-C6FH4]•

SCF (BP86) Energy = -330.785162097
Enthalpy 0K = -330.708103
Enthalpy 298K = -330.702803
Free Energy 298K = -330.737667
C 1.20621 0.29834 0.00000

C 0.00000 0.97917 0.00000
C -1.18839 0.22794 0.00000
C -1.11073 -1.17540 0.00000
C 0.13061 -1.83291 0.00000
C 1.32738 -1.07765 0.00000
F -0.05437 2.33230 0.00000
H -2.15002 0.75309 0.00000
H -2.03643 -1.76046 0.00000
H 0.18010 -2.92735 0.00000
H 2.30528 -1.57291 0.00000

[3-C6FH4]•

SCF (BP86) Energy = -330.788871026
Enthalpy 0K = -330.711888
Enthalpy 298K = -330.706595
Free Energy 298K = -330.741417
C -1.27003 -1.07659 0.00000
C -1.27348 0.30688 0.00000
C 0.00000 0.90914 0.00000
C 1.18115 0.15378 0.00000
C 1.09854 -1.24780 0.00000
C -0.15609 -1.89946 0.00000
H -2.17953 0.92014 0.00000
F 0.08465 2.26320 0.00000
H 2.14454 0.66977 0.00000
H 2.01876 -1.84294 0.00000
H -0.22617 -2.99139 0.00000

[4-C6FH4]•

SCF (BP86) Energy = -330.787216320
Enthalpy 0K = -330.710205
Enthalpy 298K = -330.704913
Free Energy 298K = -330.739727
C -1.84702 0.00000 0.00000
C -1.21425 -1.23261 0.00000
C 0.19777 -1.23026 0.00000
C 0.86963 0.00000 0.00000
C 0.19777 1.23026 0.00000
C -1.21425 1.23261 0.00000
H -1.76657 -2.17782 0.00000
H 0.77250 -2.16066 0.00000
F 2.22779 0.00000 0.00000
H 0.77250 2.16066 0.00000
H -1.76657 2.17782 0.00000

[C6H5]•

SCF (BP86) Energy = -231.554963712
Enthalpy 0K = -231.470093
Enthalpy 298K = -231.465571
Free Energy 298K = -231.498221
C 1.40695 0.00000 0.00000
C 0.77710 1.23326 0.00000
C -0.63656 1.22125 0.00000
C -1.33207 0.00000 0.00000
C -0.63656 -1.22125 0.00000
C 0.77710 -1.23326 0.00000
H 1.33177 2.17761 0.00000
H -1.18627 2.16949 0.00000
H -2.42682 0.00000 0.00000
H -1.18627 -2.16949 0.00000
H 1.33177 -2.17761 0.00000

F•

SCF (BP86) Energy = -99.7058888180
Enthalpy 0K = -99.705889
Enthalpy 298K = -99.704473
Free Energy 298K = -99.720702
F 0.00000 0.00000 0.00000

H•

SCF (BP86) Energy = -0.49810323829
Enthalpy 0K = -0.498103
Enthalpy 298K = -0.496687
Free Energy 298K = -0.508757
H 0.00000 0.00000 0.00000

Phosphines

PMe3

SCF (BP86) Energy = -126.314155220
Enthalpy 0K = -126.204440
Enthalpy 298K = -126.197551
Free Energy 298K = -126.233936
P 0.00001 -0.00005 -0.61991
C 0.00009 1.65326 0.28835
C -1.43193 -0.82650 0.28840
C 1.43184 -0.82667 0.28841
H 0.89097 2.23093 -0.00820
H -0.89063 2.23108 -0.00840
H 0.00004 1.53211 1.38578
H -1.48638 -1.88709 -0.00739
H -1.32766 -0.76498 1.38585
H -2.37769 -0.34450 -0.00915
H 2.37763 -0.34426 -0.00837
H 1.32713 -0.76606 1.38585
H 1.48654 -1.88701 -0.00826

PPh3

SCF (BP86) Energy = -701.502627402
Enthalpy 0K = -701.237103
Enthalpy 298K = -701.220606
Free Energy 298K = -701.284090
SCRf (PCM,THF) Energy = -701.50873709
P -0.00001 -0.00001 -1.25105
C -0.32759 1.64441 -0.41602
C -1.26033 -1.10582 -0.41588
C 1.58790 -0.53853 -0.41603
C 2.79466 -0.15148 -1.04074
C 4.03390 -0.51881 -0.49489
C 4.08450 -1.29538 0.67482
C 2.89103 -1.69727 1.29603
C 1.64965 -1.32060 0.75658
H 2.75973 0.43893 -1.96398
H 4.96050 -0.20764 -0.98922
H 5.05082 -1.59166 1.09654
H 2.92424 -2.30698 2.20566
H 0.72294 -1.63894 1.24489
C -1.52960 -2.34387 -1.04120
C -2.46717 -3.23344 -0.49506
C -3.16368 -2.88954 0.67558
C -2.91389 -1.65556 1.29745
C -1.96717 -0.76883 0.75770
H -1.00184 -2.60838 -1.96514
H -2.66187 -4.19104 -0.98988
H -3.90328 -3.57827 1.09756
H -3.45748 -1.37994 2.20784
H -1.77858 0.19246 1.24650
C 0.32038 2.08990 0.75536
C 0.02573 3.35328 1.29479
C -0.92079 4.18486 0.67484
C -1.56959 3.75177 -0.49364
C -1.26791 2.49495 -1.03952
H 1.06074 1.44728 1.24268
H 0.53836 3.68768 2.20345
H -1.14751 5.16983 1.09656
H -2.30376 4.39782 -0.98698
H -1.76304 2.16875 -1.96180

Silanes

Me3SiH

SCF (BP86) Energy = -124.268248825
Enthalpy 0K = -124.152084
Enthalpy 298K = -124.144455
Free Energy 298K = -124.182513
Si -0.00004 -0.00003 0.37701
C 1.24425 -1.31103 -0.22375
H 1.28050 -1.34903 -1.32612
H 2.26171 -1.08856 0.13964
H 0.96901 -2.31557 0.13943
C 0.51335 1.73301 -0.22375
H -0.18807 2.50301 0.13937
H 1.52083 1.99683 0.13978
H 0.52853 1.78336 -1.32611
C -1.75756 -0.42195 -0.22378
H -2.48971 0.31888 0.13937
H -1.80862 -0.43440 -1.32615
H -2.07386 -1.41422 0.13970
H -0.00007 -0.00001 1.89063

Me3SiF

SCF (BP86) Energy = -223.573641032
Enthalpy 0K = -223.462757
Enthalpy 298K = -223.454229
Free Energy 298K = -223.494736
Si -0.00005 -0.00003 0.03648
C 0.51985 1.72314 -0.54099
H 0.53244 1.76496 -1.64422
H -0.17986 2.49550 -0.18094
H 1.53000 1.97954 -0.18097
C -1.75201 -0.41133 -0.54170
H -2.07099 -1.40360 -0.18196
H -2.47931 0.33509 -0.18163
H -1.79426 -0.42105 -1.64493
C 1.23255 -1.31144 -0.54134
H 0.94989 -2.31460 -0.18145
H 1.26250 -1.34309 -1.64458
H 2.25121 -1.09134 -0.18127
F -0.00037 -0.00035 1.69505