Supplementary Information

Contents:

1. Table S1

Table S1. The Gibbs free energy changes of some binary and ternary adducts relative to corresponding single molecules.

Process	ΔG /kcal·mol^{-1}
$B(C_6F_5)_3$+PhHC=NPh→PhHC=PhN---$B(C_6F_5)_3$ (IM0)	-5.2
$B(C_6F_5)_3$+ H_2O→H_2O---$B(C_6F_5)_3$	-3.8
$B(C_6F_5)_3$+SiH_3Ph→PhH_2SiH---$B(C_6F_5)_3$	1.1
$B(C_6F_5)_3$+PhH_2C-NHPh→PhH_2C-N(Ph)(H)---$B(C_6F_5)_3$	-2.8
$B(C_6F_5)_3$+PhH_2C-N(SiH_2Ph)Ph→PhH_2C-N(Ph)$SiPhH_2$---$B(C_6F_5)_3$	1.4
$B(C_6F_5)_3$+H_2O+PhHC=NPh→$(C_6F_5)_3B$---O(H)-H---NPh=CHPh (IM1)	-14.4
$B(C_6F_5)_3$+H_2O+PhH_2C-NHPh→$(C_6F_5)_3B$---O(H)-H---N(H)(Ph)-CH_2Ph (IM2)	-14.4
$B(C_6F_5)_3$+2H_2O→$(C_6F_5)_3B$---O(H)H---OH_2	-8.7
$B(C_6F_5)_3$+H_2O+ PhH_2C-N(SiH_2Ph)Ph→$(C_6F_5)_3B$---O(H)-H---N(SiH_2Ph)Ph(CH_2Ph)	-7.6
$B(C_6F_5)_3$+H_2O+SiH_3Ph→$(C_6F_5)_3B$---O(H)-H---$HSiH_2Ph$	-0.5
$B(C_6F_5)_3$ +PhHC=NPh+H_2O→$(C_6F_5)_3B$---NPh=CHPh---H_2O	-2.9
$B(C_6F_5)_3$+SiH_3Ph+H_2O→$(C_6F_5)_3B$---H-Si(H_2Ph)---OH_2	5.0
$B(C_6F_5)_3$+SiH_3Ph+PhHC=NPh→$(C_6F_5)_3B$---H-Si(H_2Ph)---NPh=CHPh	6.2
H_2O+SiH_3Ph→H_2O---SiH_3Ph	2.0
SiH_3Ph+PhH_2C-NHPh→ PhH_3Si---NHPh-CH_2Ph	3.0

2. Figure S1

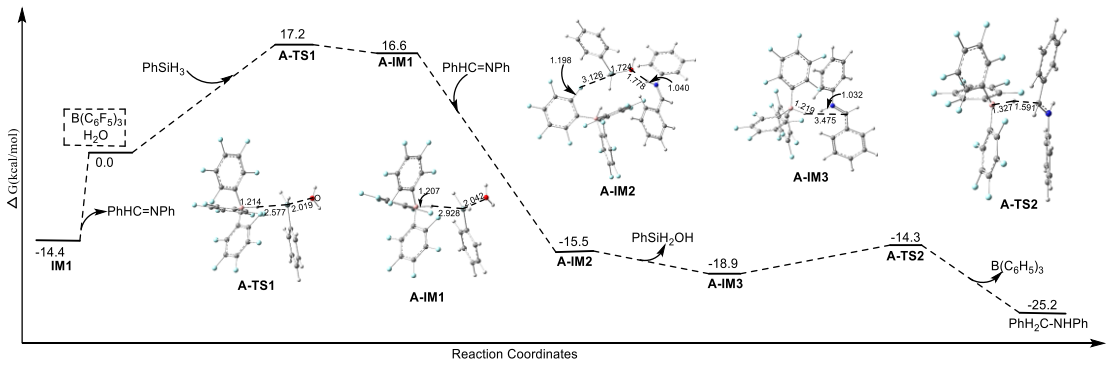

Figure S1. The Gibbs free energy profile of Path A in chloroform (unit: kcal/mol; with interatomic distances in angstroms).

3. Figure S2

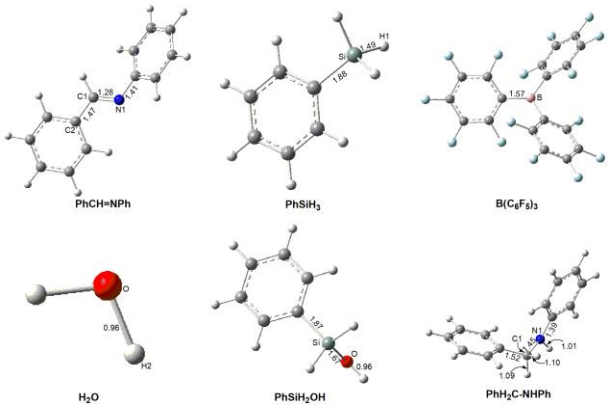

Figure S2. The opted geometries of reactants and products at B3LYP/6-311G(d,p) level in gas phase with corresponding bond lengths in angstroms.

4. Figure S3

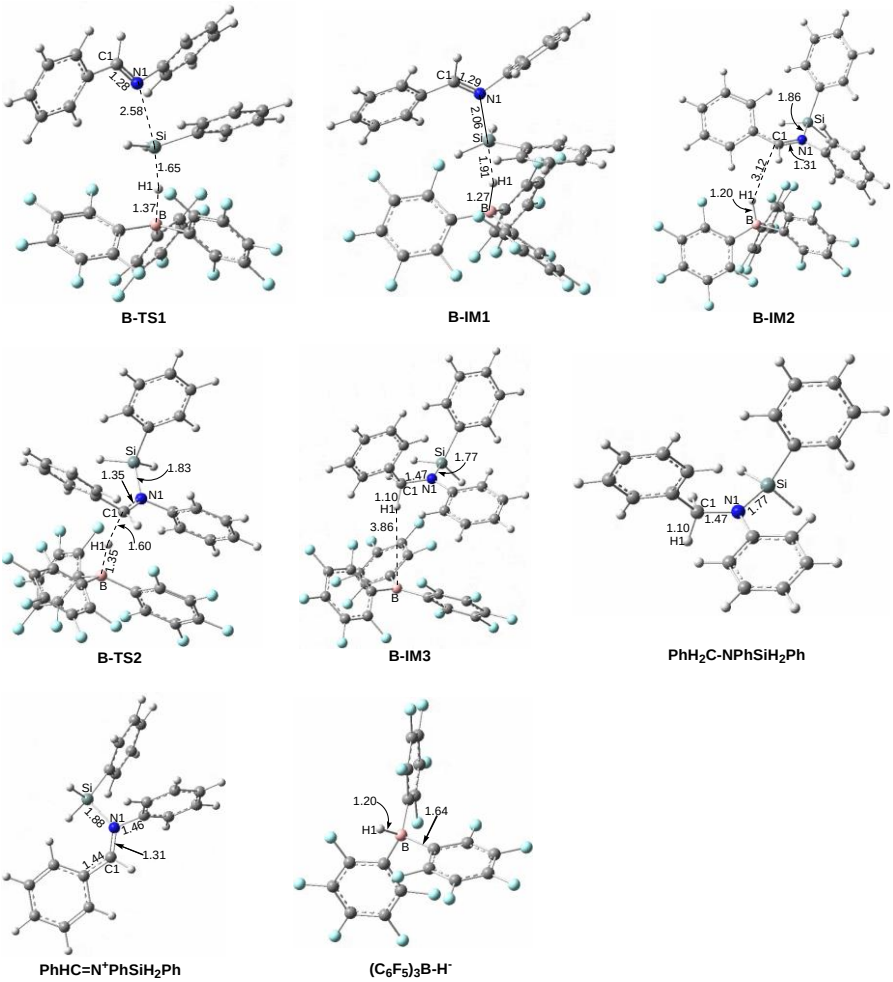

Figure S3. The opted geometries of stationary points of N-silicon amine forming steps (B-I' and B-I) at B3LYP/6-311G(d,p) level in gas phase with corresponding interatomic distances in angstroms.

5. Figure S4

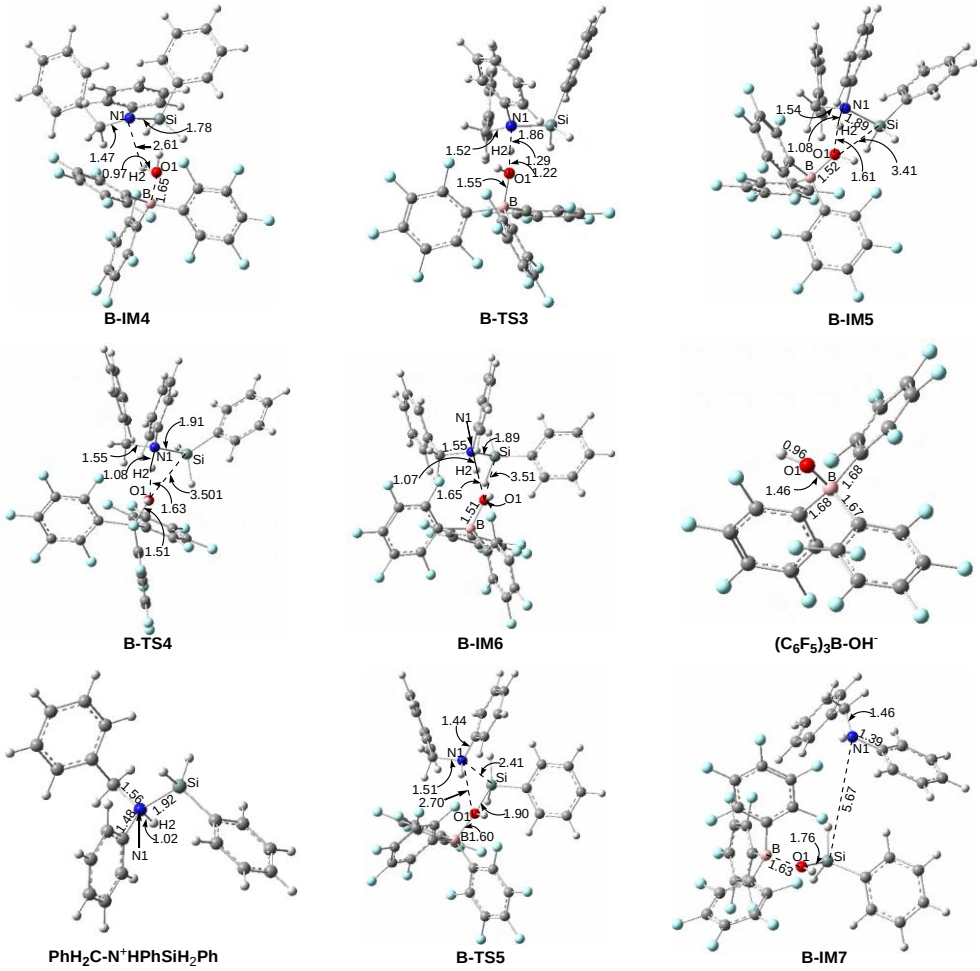

Figure S4. The opted geometries of stationary points of hydrolysis for desilylation steps (B-II) at B3LYP/6-311G(d,p) level in gas phase with corresponding interatomic distances in angstroms.

6. Optimized Cartesian coordinates of the stationary points

The following is the optimized Cartesian coordinates and the sum of electronic and thermal Gibbs free energies of the stationary points at B3LYP/6-311G(d,p) level in gas phase.

$(C_6F_5)_3B$---NPh=CHPh (IM0)

Sum of electronic and thermal Free Energies= -2765.463939 Hartree/Particle

C	-0.198104	2.653424	0.472472
C	-0.226915	1.543467	-0.366988
C	-0.542663	1.845192	-1.695757
C	-0.797492	3.125354	-2.163416
C	-0.751116	4.195710	-1.279375
C	-0.448037	3.955407	0.050633
N	-0.070933	-0.052797	0.047425
C	1.263318	-0.804636	-0.587784
C	1.585817	-2.106305	-0.196078
C	2.662497	-2.834493	-0.675661

C	3.505054	-2.256721	-1.614991
C	3.247120	-0.963248	-2.035834
C	2.155327	-0.271099	-1.519132
F	0.804921	-2.751721	0.703094
F	2.889913	-4.083577	-0.250358
F	4.552032	-2.932799	-2.093809
F	4.066615	-0.372672	-2.914966
F	2.050859	1.005207	-1.947094
F	-0.601060	0.855837	-2.608811
F	-1.084044	3.339440	-3.452643
F	-0.991260	5.438151	-1.706811
F	-0.398511	4.972815	0.921266
F	0.086341	2.525443	1.794349
C	-1.505960	-0.753619	-0.416589
C	-2.721479	-0.152963	-0.065516
C	-3.969323	-0.611801	-0.461865
C	-4.053316	-1.730342	-1.277455
C	-2.883631	-2.355335	-1.677391
C	-1.652145	-1.862485	-1.254727
F	-2.734458	0.949556	0.714712
F	-5.085537	0.014476	-0.068326
F	-5.241392	-2.193371	-1.673974
F	-2.943831	-3.427858	-2.476893
F	-0.588470	-2.535207	-1.733945
N	0.082321	-0.227510	1.705716
C	1.155888	-0.104185	2.427843
C	-1.072223	-0.625498	2.516773
C	-1.569931	-1.926402	2.466881
C	-1.626427	0.314022	3.385312
C	-2.632559	-2.280437	3.294439
H	-1.126382	-2.651507	1.801899
C	-2.692380	-0.050507	4.203914
H	-1.242696	1.325549	3.393523
C	-3.198055	-1.346598	4.160249
H	-3.015441	-3.293710	3.260661
H	-3.127883	0.684560	4.870415
H	-4.028221	-1.628738	4.797135
H	1.035104	-0.425509	3.460116
C	2.504937	0.369166	2.151419
C	3.481108	-0.058708	3.074640
C	2.891127	1.244239	1.121940
C	4.806602	0.329280	2.944069
H	3.191260	-0.710382	3.891787
C	4.214193	1.648623	1.009277

H	2.165874	1.627313	0.423407
C	5.175186	1.186284	1.908394
H	5.546388	-0.023515	3.652365
H	4.495965	2.327184	0.213182
H	6.206904	1.503094	1.808086

$(C_6F_5)_3B{-}{-}{-}OH_2$

Sum of electronic and thermal Free Energies= -2285.211959 Hartree/Particle

C	1.546679	-2.097884	1.023462
C	1.237981	-0.960165	0.287209
C	2.058362	-0.749764	-0.820834
C	3.108418	-1.594794	-1.160211
C	3.376917	-2.710082	-0.377021
C	2.584237	-2.969710	0.732974
B	-0.011343	0.016734	0.654474
C	-1.472649	-0.606505	0.278037
C	-2.621599	-0.285590	0.995223
C	-3.890992	-0.758845	0.707570
C	-4.051280	-1.611770	-0.377399
C	-2.944196	-1.958976	-1.139508
C	-1.690333	-1.457871	-0.804767
F	-2.531515	0.575327	2.063313
F	-4.944158	-0.408066	1.450500
F	-5.257439	-2.088568	-0.683586
F	-3.091898	-2.770773	-2.189217
F	-0.674500	-1.816835	-1.608783
F	1.838285	0.290211	-1.642276
F	3.859740	-1.346305	-2.235737
F	4.383372	-3.526496	-0.689080
F	2.823052	-4.038087	1.498923
F	0.790412	-2.415119	2.128655
O	0.017062	0.053357	2.329948
C	0.207172	1.578178	0.290009
C	1.305650	2.267190	0.811915
C	1.566773	3.603695	0.546734
C	0.709935	4.309671	-0.288659
C	-0.387390	3.666398	-0.842507
C	-0.618053	2.326805	-0.548250
F	2.185995	1.626686	1.605720
F	2.631775	4.213700	1.078292
F	0.942972	5.594876	-0.557769
F	-1.213351	4.337333	-1.652425
F	-1.693702	1.770806	-1.137895
H	0.152800	-0.843023	2.685812

H	-0.827755	0.404386	2.660657

PhH_2SiH---$B(C_6F_5)_3$

Sum of electronic and thermal Free Energies= -2731.699548 Hartree/Particle

C	0.191763	2.370353	-0.228295
C	1.185672	1.544533	0.305032
C	2.329143	2.197581	0.776281
C	2.478462	3.576047	0.737413
C	1.464967	4.354599	0.189055
C	0.314526	3.748955	-0.304001
B	1.024548	-0.015427	0.370244
C	-0.350808	-0.637437	0.784817
C	-0.872278	-1.775969	0.159054
C	-2.096631	-2.327891	0.500330
C	-2.836057	-1.756529	1.529276
C	-2.359474	-0.626176	2.182369
C	-1.142900	-0.084443	1.797858
F	-0.201157	-2.357838	-0.848194
F	-2.574178	-3.392461	-0.149382
F	-4.001872	-2.287117	1.885302
F	-3.076646	-0.074901	3.164876
F	-0.720371	1.001044	2.467538
F	3.330478	1.489986	1.323502
F	3.578452	4.160681	1.217421
F	1.596504	5.677124	0.135423
F	-0.655395	4.495121	-0.839412
F	-0.934503	1.831976	-0.728964
C	2.238681	-0.940824	0.017622
C	3.130034	-0.636904	-1.018332
C	4.203706	-1.449092	-1.350626
C	4.430941	-2.608160	-0.616968
C	3.579660	-2.946701	0.429093
C	2.502868	-2.122947	0.719815
F	2.948513	0.464521	-1.763777
F	5.017552	-1.131994	-2.360285
F	5.462277	-3.392788	-0.915494
F	3.806713	-4.055153	1.137723
F	1.718520	-2.488538	1.745647
H	-1.564846	-0.633033	-2.955076
Si	-2.859348	-0.025667	-3.366422
H	-3.418216	-0.850259	-4.469064
H	-2.591021	1.350116	-3.857113
C	-4.076651	0.024302	-1.931379
C	-4.920860	-1.066708	-1.667864

C	-4.152455	1.138113	-1.080054
C	-5.802095	-1.050361	-0.589142
H	-4.894445	-1.940596	-2.311319
C	-5.032757	1.156861	0.000520
H	-3.515746	1.998654	-1.255341
C	-5.858073	0.061959	0.248448
H	-6.441857	-1.905076	-0.400825
H	-5.075743	2.026279	0.647325
H	-6.540270	0.074424	1.090867

PhH_2C-(H) (Ph)N---$B(C_6F_5)_3$

Sum of electronic and thermal Free Energies= -2766.656916 Hartree/Particle

C	1.672938	-0.279484	2.374638
C	1.528582	-0.490168	1.009606
C	2.667553	-1.035764	0.404243
C	3.826945	-1.376433	1.082540
C	3.901706	-1.161878	2.452893
C	2.811957	-0.608079	3.103045
B	0.307618	-0.068226	-0.009340
C	-0.311584	-1.333452	-0.873131
C	-1.272689	-1.117839	-1.861850
C	-1.867980	-2.106067	-2.624377
C	-1.512731	-3.429331	-2.398363
C	-0.591005	-3.715938	-1.404812
C	-0.027830	-2.683018	-0.659027
F	-1.713993	0.153224	-2.096289
F	-2.785254	-1.803570	-3.551074
F	-2.068046	-4.409716	-3.113577
F	-0.260953	-4.987834	-1.152990
F	0.806680	-3.079854	0.319636
F	2.665719	-1.268731	-0.924563
F	4.869071	-1.906567	0.432928
F	5.006665	-1.482859	3.130155
F	2.860780	-0.381786	4.422151
F	0.674593	0.282234	3.104171
C	0.948590	1.165352	-0.931347
C	1.546137	2.276211	-0.319941
C	2.181938	3.310006	-0.994074
C	2.287655	3.253783	-2.375057
C	1.765549	2.154918	-3.037671
C	1.131366	1.143525	-2.321350
F	1.554566	2.394565	1.030727
F	2.701963	4.343893	-0.322354
F	2.894122	4.231044	-3.050247

F	1.887374	2.064028	-4.366405
F	0.735199	0.103231	-3.072845
N	-1.186510	0.527660	0.686954
H	-1.600543	0.835758	-0.194245
C	-1.275660	1.780277	1.569702
H	-0.469489	2.437290	1.270861
H	-1.091768	1.465880	2.590165
C	-2.119924	-0.509070	1.187470
C	-1.778975	-1.327567	2.260106
C	-3.368849	-0.632435	0.580723
C	-2.691669	-2.276790	2.715349
H	-0.820874	-1.230546	2.744404
C	-4.274089	-1.585233	1.040081
H	-3.636041	0.008194	-0.251384
C	-3.937800	-2.411097	2.108987
H	-2.418218	-2.916330	3.546251
H	-5.240774	-1.677053	0.559357
H	-4.640721	-3.154468	2.466003
C	-2.603292	2.483735	1.430853
C	-3.595825	2.352512	2.406042
C	-2.850433	3.300896	0.321061
C	-4.812332	3.017357	2.272678
H	-3.414439	1.727017	3.273164
C	-4.068879	3.959519	0.181077
H	-2.080592	3.433439	-0.433548
C	-5.052568	3.818165	1.158374
H	-5.571743	2.909897	3.038627
H	-4.245334	4.591013	-0.681999
H	-5.999172	4.336022	1.054749

PhH_2C-N(Ph)$SiPhH_2$---$B(C_6F_5)_3$

Sum of electronic and thermal Free Energies= -3288.429081 Hartree/Particle

C	-2.488311	-2.975943	0.158586
C	-2.370826	-1.683989	-0.368654
C	-2.259783	-1.604327	-1.762503
C	-2.249381	-2.722266	-2.582322
C	-2.379829	-3.983738	-2.011872
C	-2.505870	-4.113802	-0.633090
B	-2.353706	-0.412347	0.543499
C	-3.065020	0.905425	0.078594
C	-2.501313	2.168255	0.289750
C	-3.095073	3.342281	-0.146261
C	-4.324733	3.282801	-0.792207
C	-4.935975	2.052019	-1.005930

C	-4.298363	0.895436	-0.582576
F	-1.308118	2.284394	0.898485
F	-2.497253	4.522171	0.043405
F	-4.914996	4.400346	-1.205199
F	-6.121687	1.997180	-1.616253
F	-4.930913	-0.266314	-0.809215
F	-2.119446	-0.411593	-2.361756
F	-2.118891	-2.601873	-3.904681
F	-2.384961	-5.065418	-2.784351
F	-2.641172	-5.325670	-0.089810
F	-2.623170	-3.154394	1.482562
C	-1.610464	-0.446579	1.925174
C	-2.139263	0.153824	3.072253
C	-1.488091	0.143265	4.297231
C	-0.241349	-0.464261	4.398879
C	0.325707	-1.068503	3.282647
C	-0.365255	-1.063436	2.081398
F	-3.340699	0.751002	3.025046
F	0.236928	-1.645489	1.031348
F	1.535752	-1.633798	3.373371
F	0.406136	-0.468415	5.560271
F	-2.038954	0.712334	5.371640
H	2.841586	1.362271	0.596146
C	3.208257	0.342105	0.430891
N	2.995331	0.036465	-0.993005
Si	1.751777	0.993630	-1.787350
C	3.364854	-1.257788	-1.454882
C	3.386165	-2.375693	-0.607546
C	3.755823	-3.627698	-1.092912
C	4.103746	-3.800859	-2.429216
C	4.090554	-2.694932	-3.277375
C	3.739494	-1.439158	-2.795887
H	3.109339	-2.276136	0.433258
H	3.767229	-4.474179	-0.414790
H	4.390146	-4.777273	-2.802032
H	4.373771	-2.804269	-4.318622
H	3.765889	-0.583673	-3.459941
C	2.199728	2.817761	-1.821148
C	1.362017	3.773228	-1.225270
C	1.668456	5.132465	-1.277729
C	2.821925	5.560812	-1.928961
C	3.668862	4.627645	-2.526529
C	3.359671	3.271898	-2.471325
H	0.462882	3.456426	-0.707019

H	1.007583	5.853246	-0.809036
H	3.062610	6.617345	-1.970747
H	4.568502	4.958032	-3.034067
H	4.030363	2.559977	-2.942748
H	2.601085	-0.302987	1.077531
C	4.655075	0.283485	0.890338
C	4.962887	-0.217612	2.157306
C	5.690518	0.772343	0.089941
C	6.276709	-0.222223	2.622072
H	4.168520	-0.611024	2.784311
C	7.004133	0.764838	0.549822
H	5.460606	1.151908	-0.898357
C	7.302019	0.269330	1.818455
H	6.498691	-0.617428	3.607240
H	7.798160	1.145418	-0.083371
H	8.326041	0.261750	2.174710
H	1.575596	0.448648	-3.151551
H	0.454559	0.898945	-1.053096

$(C_6F_5)_3B$---O(H)-H---NPh=CHPh (IM1)

Sum of electronic and thermal Free Energies=-2841.936214 Hartree/Particle

N	-0.745537	-0.344597	0.017848
C	-1.723438	-1.338669	-0.835760
C	-3.106663	-1.425313	-0.684540
C	-1.194219	-2.179995	-1.817025
C	-3.911269	-2.260234	-1.455050
C	-1.958047	-3.022787	-2.609555
C	-3.334625	-3.060955	-2.428211
C	-1.558240	0.858362	0.788893
C	-2.016177	1.993896	0.131705
C	-1.871603	0.818729	2.147091
C	-2.681479	3.044324	0.745326
C	-2.549437	1.837435	2.806967
C	-2.949117	2.966322	2.104294
C	0.349464	-1.068614	0.985287
C	0.378790	-2.426562	1.300033
C	1.347684	-0.310770	1.595899
C	1.339818	-2.994950	2.130029
C	2.330961	-0.835782	2.419874
C	2.327484	-2.197051	2.688599
F	-2.817228	1.742854	4.113484
F	-3.585923	3.961908	2.725569
F	-3.047242	4.129828	0.046416
F	-1.821317	2.126024	-1.220045

F	-1.542590	-0.252284	2.892316
F	-1.384572	-3.804313	-3.534280
F	-4.091355	-3.865615	-3.178954
F	0.142203	-2.231856	-2.014488
F	-3.753626	-0.694377	0.245583
F	-5.236034	-2.293336	-1.264686
F	1.393491	1.030253	1.392450
F	3.280741	-0.049080	2.944435
F	3.263706	-2.731771	3.476924
F	1.321279	-4.307356	2.392507
F	-0.550797	-3.272380	0.820019
O	0.144056	0.367516	-1.129565
H	1.153850	0.632098	-1.087810
H	-0.352706	1.039892	-1.616060
N	2.687631	1.005335	-1.264728
C	3.162141	2.145007	-1.618571
C	3.586176	-0.082584	-1.078692
C	4.756758	0.063629	-0.324934
C	3.259662	-1.327764	-1.626166
C	5.606809	-1.024228	-0.146858
H	4.970999	1.009980	0.157446
C	4.122702	-2.404282	-1.453638
H	2.342266	-1.441782	-2.188041
C	5.297273	-2.257358	-0.715993
H	6.503296	-0.909658	0.451274
H	3.870017	-3.363765	-1.889421
H	5.958427	-3.103726	-0.572029
H	4.225065	2.224945	-1.864668
C	2.381551	3.373422	-1.764698
C	2.871309	4.373711	-2.618838
C	1.175324	3.589437	-1.079728
C	2.147937	5.542978	-2.822085
H	3.814142	4.223088	-3.134082
C	0.456620	4.761068	-1.282130
H	0.834280	2.860258	-0.357086
C	0.936565	5.734387	-2.159536
H	2.527885	6.304381	-3.492964
H	-0.478567	4.918106	-0.758269
H	0.371952	6.646349	-2.315092

$(C_6F_5)_3B$---O(H)-H--- NHPh(CH_2Ph) (IM2)

Sum of electronic and thermal Free Energies= -2843.125234 Hartree/Particle

C	-3.407605	0.309545	1.901759
N	-2.498389	1.337037	1.307657

C	-2.419770	2.609473	1.962599
C	-2.208976	3.758656	1.190321
C	-2.059841	4.997234	1.806093
C	-2.119455	5.106980	3.194176
C	-2.325647	3.963297	3.960556
C	-2.472303	2.716948	3.355038
H	-2.877770	-0.205522	2.702491
H	-2.159938	3.679990	0.108825
H	-1.902780	5.878826	1.195376
H	-2.006343	6.072695	3.671740
H	-2.370131	4.034672	5.041233
H	-2.617352	1.836233	3.967697
H	-2.765816	1.475737	0.337019
H	-4.277484	0.812818	2.338626
C	-3.856346	-0.677563	0.848722
C	-3.316353	-1.964428	0.783210
C	-4.819941	-0.300006	-0.094899
C	-3.719364	-2.851499	-0.213214
H	-2.576510	-2.268810	1.513250
C	-5.220959	-1.183800	-1.093240
H	-5.269544	0.687514	-0.041494
C	-4.667508	-2.461790	-1.155757
H	-3.284649	-3.842971	-0.257603
H	-5.966821	-0.878109	-1.817947
H	-4.973365	-3.148934	-1.935620
O	0.158603	0.975599	1.069423
B	0.850724	-0.004693	-0.021373
C	2.271551	0.743572	-0.336278
C	3.119374	1.104398	0.714403
C	2.769704	1.013457	-1.611085
C	4.357733	1.707102	0.531941
C	4.003819	1.612036	-1.836071
C	4.802523	1.964756	-0.757197
C	-0.213434	-0.038319	-1.265957
C	-0.740939	-1.180566	-1.863549
C	-0.704249	1.160182	-1.783102
C	-1.681138	-1.138515	-2.890108
C	-1.645583	1.252660	-2.794195
C	-2.142726	0.082429	-3.355392
C	1.097546	-1.431716	0.725817
C	0.412715	-1.872670	1.851612
C	2.056324	-2.323092	0.244242
C	0.652455	-3.090046	2.476164
C	2.336086	-3.546573	0.837566

C	1.628991	-3.933640	1.968648
H	0.369935	1.895044	0.858478
F	5.121304	2.036558	1.580778
F	5.988248	2.544183	-0.957597
F	4.429490	1.849043	-3.082377
F	2.752632	0.865559	1.990756
F	2.070048	0.678999	-2.711205
F	-0.257555	2.342817	-1.269914
F	-2.088480	2.445201	-3.216863
F	-3.063560	0.136148	-4.320345
F	-2.164058	-2.271388	-3.412424
F	-0.372137	-2.410527	-1.463611
F	3.268425	-4.358342	0.326295
F	2.745086	-2.027453	-0.875652
F	1.875950	-5.109939	2.551135
F	-0.064960	-3.458055	3.547445
F	-0.584314	-1.124240	2.393383
H	-0.860321	0.932138	1.180625

$(C_6F_5)_3B$---O(H)H---OH_2

Sum of electronic and thermal Free Energies= -2361.661887 Hartree/Particle

B	-0.014010	-0.016617	0.546754
C	-0.902893	-1.354388	0.269552
C	-0.561032	-2.362326	-0.632044
C	-2.127621	-1.535262	0.918321
C	-1.356727	-3.478661	-0.864518
C	-2.947482	-2.637538	0.718266
C	-2.556163	-3.619827	-0.181586
C	1.542398	-0.110419	0.060358
C	2.423921	-1.001303	0.670909
C	2.096653	0.633738	-0.979306
C	3.752692	-1.156322	0.312293
C	3.425125	0.513230	-1.376877
C	4.259598	-0.383493	-0.725452
C	-0.774756	1.365643	0.145813
C	-1.725872	1.446165	-0.871508
C	-0.492707	2.577977	0.764119
C	-2.365797	2.628750	-1.226238
C	-1.104989	3.781499	0.450775
C	-2.058834	3.805244	-0.557120
F	3.904303	1.255767	-2.380337
F	5.536592	-0.506032	-1.092337
F	4.542121	-2.031452	0.944125
F	1.973180	-1.811248	1.672999

F	1.349486	1.509284	-1.676620
F	-4.107475	-2.757601	1.374728
F	-3.328679	-4.687614	-0.390108
F	-2.579847	-0.601138	1.779484
F	0.572620	-2.289461	-1.355098
F	-0.976464	-4.415605	-1.740304
F	0.459686	2.631216	1.740051
F	-0.782169	4.907164	1.100695
F	-2.666190	4.947727	-0.883610
F	-3.271445	2.642885	-2.209458
F	-2.055133	0.359288	-1.593213
O	0.071295	-0.010594	2.197706
H	0.748564	0.589253	2.623372
H	0.317595	-0.906732	2.471123
O	2.008138	1.238982	3.507846
H	2.214359	2.084818	3.093283
H	1.865715	1.433775	4.440537

$(C_6F_5)_3B$---O(H)-H---N(SiH_2Ph)Ph(CH_2Ph)

Sum of electronic and thermal Free Energies= -3364.879404 Hartree/Particle

C	-3.548369	2.044999	0.300425
N	-3.252785	0.654322	-0.072493
C	-2.581240	0.423036	-1.282818
C	-2.353607	-0.894085	-1.736226
C	-1.672556	-1.143987	-2.921727
C	-1.193887	-0.095141	-3.708426
C	-1.423996	1.211795	-3.282720
C	-2.100284	1.474789	-2.092619
H	-3.871361	2.038217	1.343829
H	-2.739607	-1.736444	-1.176268
H	-1.523524	-2.171434	-3.233035
H	-0.680960	-0.291865	-4.642197
H	-1.079504	2.046658	-3.882977
H	-2.280062	2.503398	-1.816449
H	-2.630433	2.644132	0.285386
C	-4.624308	2.742364	-0.521885
C	-4.712735	4.137557	-0.468577
C	-5.553753	2.040164	-1.290116
C	-5.714885	4.815090	-1.156916
H	-3.991819	4.698276	0.119352
C	-6.555500	2.717488	-1.984585
H	-5.484823	0.961310	-1.357118
C	-6.641973	4.105288	-1.918584
H	-5.769196	5.896741	-1.102982

H	-7.266347	2.157163	-2.581840
H	-7.420345	4.630990	-2.459802
O	1.131869	0.472832	-1.301253
B	2.125824	0.012220	-0.049725
C	3.523134	-0.271719	-0.822653
C	4.069912	0.701417	-1.663306
C	4.278765	-1.436605	-0.697322
C	5.262188	0.534350	-2.353688
C	5.479836	-1.640129	-1.367946
C	5.972715	-0.649724	-2.205060
C	1.392007	-1.290736	0.601745
C	1.219201	-1.509553	1.967020
C	0.861801	-2.284775	-0.216359
C	0.542096	-2.612129	2.480312
C	0.167763	-3.390080	0.243861
C	0.004727	-3.551812	1.613111
C	2.146236	1.318909	0.922935
C	1.006529	2.068292	1.188197
C	3.288418	1.749964	1.596810
C	0.965286	3.174005	2.022030
C	3.299872	2.849284	2.448394
C	2.132467	3.571105	2.659810
H	0.925076	-0.251655	-1.916250
F	5.735362	1.500325	-3.149976
F	7.122054	-0.830564	-2.858639
F	6.162469	-2.780321	-1.212463
F	3.444793	1.884711	-1.822137
F	3.879729	-2.436465	0.112290
F	1.020325	-2.188301	-1.568623
F	-0.362125	-4.279464	-0.605142
F	-0.688830	-4.591724	2.085912
F	0.390964	-2.764021	3.799584
F	1.717467	-0.648332	2.872624
F	4.425005	3.216228	3.068691
F	4.449489	1.084545	1.469765
F	2.130312	4.630419	3.470451
F	-0.175348	3.849159	2.214640
F	-0.182779	1.712320	0.608207
H	0.288038	0.879546	-1.031478
H	-3.853270	0.127602	2.367920
H	-2.137045	-1.289431	1.372497
Si	-3.441678	-0.613966	1.153197
C	-4.690117	-1.959029	0.752745
C	-4.308475	-3.309588	0.793193

C	-6.031343	-1.659092	0.461649
C	-5.231650	-4.324809	0.548239
H	-3.281117	-3.578949	1.019301
C	-6.954800	-2.670696	0.214025
H	-6.363465	-0.626045	0.430354
C	-6.555239	-4.005911	0.256428
H	-4.916426	-5.361536	0.584750
H	-7.985772	-2.419294	-0.009053
H	-7.274506	-4.794237	0.064383

$(C_6F_5)_3B$---O(H)-H---$HSiH_2Ph$

Sum of electronic and thermal Free Energies= -2808.146705 Hartree/Particle

B	0.766299	-0.058462	-0.105899
C	0.944869	-1.646535	0.157083
C	0.802498	-2.273320	1.394411
C	1.290757	-2.492662	-0.900451
C	0.974515	-3.641188	1.577690
C	1.465987	-3.861739	-0.759203
C	1.304853	-4.440859	0.493311
C	0.059231	0.787643	1.099104
C	-1.300747	0.683845	1.374050
C	0.753941	1.638678	1.958124
C	-1.957353	1.368588	2.382024
C	0.144055	2.342293	2.992229
C	-1.221891	2.213154	3.203482
C	2.060787	0.682746	-0.757895
C	3.371273	0.299168	-0.474604
C	1.952042	1.778760	-1.606047
C	4.483107	0.943417	-1.004103
C	3.026526	2.452660	-2.165514
C	4.311175	2.024863	-1.858466
F	0.862546	3.143274	3.783098
F	-1.821546	2.888982	4.183093
F	-3.276803	1.231613	2.563135
F	-2.081012	-0.153782	0.615190
F	2.082848	1.800095	1.836350
F	1.792972	-4.623891	-1.808670
F	1.469446	-5.755019	0.651657
F	1.487949	-1.983885	-2.132093
F	0.498987	-1.565020	2.499313
F	0.823412	-4.190243	2.788015
F	0.707242	2.256683	-1.938454
F	2.838714	3.492923	-2.983054
F	5.369064	2.649661	-2.376401

F	5.716556	0.534416	-0.695327
F	3.615427	-0.717888	0.369152
O	-0.344981	-0.044924	-1.353872
H	-0.389394	0.827970	-1.784304
H	-1.231721	-0.272940	-1.027466
H	-2.603844	1.735551	-1.836745
Si	-4.021377	2.142809	-1.589033
H	-4.387208	3.102806	-2.659657
H	-4.049286	2.810195	-0.263851
C	-5.160701	0.651981	-1.618299
C	-5.352879	-0.134123	-0.470076
C	-5.831374	0.283527	-2.795316
C	-6.181586	-1.253140	-0.501205
H	-4.856411	0.127982	0.458322
C	-6.660121	-0.835733	-2.827699
H	-5.713737	0.877988	-3.696036
C	-6.835310	-1.605955	-1.680195
H	-6.320414	-1.846338	0.395754
H	-7.171860	-1.103039	-3.745521
H	-7.482610	-2.475494	-1.703171

$(C_6F_5)_3B$---NPh=CHPh---H_2O

Sum of electronic and thermal Free Energies= -2841.903712 Hartree/Particle

C	0.238806	2.779568	0.539551
C	0.060715	1.713770	-0.337714
C	-0.191199	2.100537	-1.657735
C	-0.252003	3.418195	-2.084205
C	-0.062214	4.441374	-1.164073
C	0.185631	4.116939	0.159511
B	-0.018737	0.100015	0.023617
C	1.220084	-0.804555	-0.614084
C	1.378847	-2.143302	-0.251201
C	2.353490	-2.993708	-0.746054
C	3.271467	-2.507912	-1.665984
C	3.184879	-1.180927	-2.051644
C	2.185520	-0.367321	-1.523722
F	0.518282	-2.712316	0.633230
F	2.403122	-4.274657	-0.356066
F	4.224153	-3.301432	-2.159381
F	4.080660	-0.677824	-2.909430
F	2.253356	0.921038	-1.917526
F	-0.380880	1.158804	-2.603671
F	-0.487835	3.712929	-3.367801
F	-0.114044	5.718500	-1.551403

F	0.370143	5.087713	1.064232
F	0.480217	2.568718	1.858911
C	-1.525905	-0.386562	-0.486218
C	-2.653660	0.383235	-0.169705
C	-3.949500	0.081266	-0.563858
C	-4.183275	-1.058145	-1.319757
C	-3.104071	-1.847984	-1.673640
C	-1.819398	-1.497119	-1.277024
F	-2.529331	1.493820	0.586519
F	-4.972277	0.867503	-0.208528
F	-5.421664	-1.387239	-1.691893
F	-3.301395	-2.980534	-2.372651
F	-0.857957	-2.342168	-1.710679
N	0.054303	-0.152043	1.671901
C	1.109964	-0.212799	2.427323
C	-1.175083	-0.399967	2.433750
C	-1.873721	-1.600016	2.307400
C	-1.596443	0.578853	3.333822
C	-3.001760	-1.812029	3.096355
H	-1.566001	-2.364363	1.609356
C	-2.729555	0.355728	4.112163
H	-1.055812	1.513985	3.398443
C	-3.433263	-0.839829	3.996548
H	-3.537629	-2.748670	2.998286
H	-3.060360	1.121765	4.803606
H	-4.314853	-1.012820	4.602795
H	0.909720	-0.548670	3.442261
C	2.522330	0.065311	2.204037
C	3.396002	-0.536373	3.132835
C	3.065143	0.910166	1.220746
C	4.767780	-0.345410	3.051197
H	2.988084	-1.167013	3.915316
C	4.436212	1.117304	1.157837
H	2.426049	1.422929	0.521037
C	5.290548	0.484555	2.061001
H	5.425109	-0.829808	3.763023
H	4.839529	1.776088	0.398213
H	6.360238	0.648453	1.999729
H	-2.310778	-4.374719	-0.663079
O	-1.934115	-4.421406	0.222191
H	-0.995968	-4.254445	0.082563

$(C_6F_5)_3B$---H-Si(H_2Ph)---OH_2

Sum of electronic and thermal Free Energies= -2808.125493 Hartree/Particle

H	-0.233761	-0.000361	-1.022303
Si	-0.856281	-0.103677	-2.489757
H	-0.223044	1.090350	-3.071801
O	-1.474605	-0.276796	-4.977637
H	-2.369685	-0.620957	-5.076657
C	-2.700438	-0.001375	-2.213175
C	-3.358594	1.238332	-2.151560
C	-3.467970	-1.172611	-2.093662
C	-4.739055	1.303556	-1.982261
H	-2.790957	2.159021	-2.220949
C	-4.848811	-1.105843	-1.922204
H	-2.986041	-2.143562	-2.116805
C	-5.485742	0.132247	-1.867902
H	-5.230727	2.268526	-1.932359
H	-5.423892	-2.019245	-1.821861
H	-6.559937	0.184388	-1.730716
H	-0.346387	-1.431835	-2.856786
H	-1.473705	0.567687	-5.441753
B	0.502821	-0.001487	0.212854
C	1.086592	1.499774	0.222485
C	0.315926	2.592581	-0.165960
C	2.378161	1.811549	0.646708
C	0.775494	3.900219	-0.174384
C	2.876987	3.109404	0.667291
C	2.072292	4.160509	0.249626
C	-0.714192	-0.330026	1.210921
C	-1.025884	0.416815	2.346281
C	-1.544394	-1.425611	0.978595
C	-2.093546	0.109637	3.183425
C	-2.627107	-1.757947	1.775647
C	-2.902056	-0.980630	2.893990
C	1.578606	-1.170313	-0.048763
C	2.332050	-1.206315	-1.220243
C	1.868639	-2.176858	0.871389
C	3.288249	-2.171804	-1.495086
C	2.825920	-3.158675	0.642251
C	3.537892	-3.158375	-0.549461
F	2.538295	5.411147	0.258446
F	4.122348	3.354203	1.088730
F	3.205926	0.847302	1.088857
F	-0.961925	2.395824	-0.570156
F	-0.013159	4.904291	-0.578382
F	1.236337	-2.224700	2.058179
F	3.069914	-4.100373	1.560323

F	4.456716	-4.097345	-0.784977
F	3.968606	-2.160266	-2.647181
F	2.132664	-0.258587	-2.167349
F	-0.279470	1.479076	2.699250
F	-2.348041	0.855737	4.264268
F	-3.935718	-1.281105	3.683270
F	-3.403098	-2.808480	1.480633
F	-1.307766	-2.220076	-0.091497

$(C_6F_5)_3B$---H-Si(H_2Ph)---NPh=CHPh

Sum of electronic and thermal Free Energies= -3288.398243 Hartree/Particle

C	1.681920	-1.398555	2.132871
C	2.073900	-0.143249	1.669038
C	2.714009	0.663392	2.610739
C	2.938606	0.262471	3.922813
C	2.510776	-0.990833	4.338917
C	1.871507	-1.831350	3.435589
B	1.834490	0.311757	0.152780
C	2.459185	-0.580418	-1.017597
C	3.561230	-1.419961	-0.851486
C	4.084342	-2.191650	-1.882848
C	3.496644	-2.146421	-3.139800
C	2.398904	-1.321809	-3.354288
C	1.920970	-0.554882	-2.304730
F	4.189755	-1.502315	0.334438
F	5.147683	-2.975199	-1.675458
F	3.982446	-2.888411	-4.135728
F	1.819836	-1.275828	-4.559241
F	0.858467	0.239302	-2.563954
F	3.174212	1.880945	2.270746
F	3.564489	1.070516	4.784479
F	2.713573	-1.387472	5.595818
F	1.454198	-3.040720	3.826246
F	1.066548	-2.256781	1.289630
C	1.643391	1.879876	-0.116988
C	0.643290	2.615694	0.517217
C	0.454280	3.975134	0.326947
C	1.305995	4.665204	-0.526152
C	2.330327	3.981692	-1.167058
C	2.479739	2.615589	-0.956904
F	-0.211944	1.993342	1.360046
F	-0.539310	4.625739	0.949454
F	1.142530	5.974091	-0.722834
F	3.162847	4.641770	-1.978087

F	3.505342	2.021465	-1.591499
H	0.374218	-0.157130	-0.024444
Si	-1.143448	-0.502947	-0.114242
N	-4.581684	-0.124308	0.652054
C	-1.337115	-2.036229	-1.151264
C	-1.358278	-3.308319	-0.555289
C	-1.514599	-4.453500	-1.330361
C	-1.649494	-4.346963	-2.713315
C	-1.632097	-3.092935	-3.321352
C	-1.479524	-1.946559	-2.546808
H	-1.252098	-3.406375	0.518901
H	-1.532141	-5.427741	-0.855416
H	-1.768578	-5.240004	-3.316753
H	-1.734751	-3.007586	-4.397151
H	-1.464339	-0.978044	-3.033782
C	-5.437579	0.623971	0.069734
C	-4.901191	-1.469502	0.925909
C	-5.525443	-2.310674	-0.006947
C	-5.790436	-3.638914	0.314783
C	-5.443257	-4.145103	1.565386
C	-4.810335	-3.315707	2.491784
C	-4.525460	-1.993561	2.170991
H	-5.767861	-1.931159	-0.992903
H	-6.262843	-4.282297	-0.419186
H	-5.652434	-5.179447	1.812492
H	-4.531444	-3.702975	3.465435
H	-4.028988	-1.340959	2.879298
H	-1.704612	0.700015	-0.755974
H	-1.514040	-0.693285	1.298987
H	-6.435170	0.246730	-0.194020
C	-5.187765	2.028767	-0.271675
C	-4.023846	2.698574	0.137727
C	-6.147651	2.726491	-1.017283
C	-3.825584	4.029721	-0.202599
H	-3.292567	2.164870	0.730739
C	-5.945671	4.059558	-1.361838
H	-7.054141	2.217625	-1.329466
C	-4.784093	4.712307	-0.955922
H	-2.925393	4.538144	0.121684
H	-6.693202	4.588197	-1.942095
H	-4.625603	5.751962	-1.219393

H_2O---SiH_3Ph

Sum of electronic and thermal Free Energies= -599.381769 Hartree/Particle

H	-1.145196	2.925497	0.002003
Si	-1.456601	1.472183	0.000225
H	-2.291050	1.173180	1.197165
O	-3.152202	-1.678089	-0.000417
H	-3.466350	-1.177875	0.759823
C	0.150415	0.500548	-0.000107
C	1.381970	1.173535	-0.000300
C	0.158041	-0.905074	0.000162
C	2.584801	0.469093	-0.000226
H	1.406259	2.258693	-0.000474
C	1.360108	-1.607845	0.000237
H	-0.781431	-1.449018	0.000239
C	2.574731	-0.923188	0.000053
H	3.526508	1.007073	-0.000372
H	1.348428	-2.692364	0.000445
H	3.509324	-1.473464	0.000140
H	-2.290250	1.176441	-1.198109
H	-3.466608	-1.176425	-0.759600

PhH_3Si---NHPh-CH_2Ph

Sum of electronic and thermal Free Energies= -1080.850285 Hartree/Particle

H	0.386583	3.398417	3.286112
Si	0.111244	2.244150	2.389612
H	1.172296	1.227785	2.624263
C	0.088509	2.821514	0.598631
C	0.938909	3.849138	0.160181
C	-0.768243	2.226400	-0.341265
C	0.940649	4.263486	-1.169884
H	1.604444	4.339696	0.864269
C	-0.770527	2.641414	-1.671958
H	-1.443002	1.433658	-0.036586
C	0.084893	3.659072	-2.088783
H	1.603989	5.060682	-1.487350
H	-1.445431	2.172629	-2.379678
H	0.081300	3.983834	-3.123499
H	-1.198008	1.641278	2.746773
N	-0.480426	-1.577190	0.201392
C	-1.868225	-1.597247	0.102410
C	-2.534710	-1.587327	-1.134793
C	-3.927683	-1.553284	-1.184422
C	-4.688289	-1.536740	-0.020229
C	-4.031115	-1.554599	1.211898
C	-2.646022	-1.582907	1.276919
C	0.375371	-1.897387	-0.938500

C	1.829442	-1.911579	-0.524906
C	2.517724	-3.118051	-0.378145
C	3.853932	-3.131784	0.020496
C	4.514994	-1.934424	0.279617
C	3.835443	-0.724539	0.138838
C	2.502023	-0.713220	-0.259568
H	0.108422	-2.867020	-1.384893
H	-1.971385	-1.608009	-2.058737
H	-4.418336	-1.546030	-2.151929
H	-5.770313	-1.513662	-0.067424
H	-4.604178	-1.545296	2.132778
H	-2.147887	-1.588367	2.241519
H	2.005984	-4.053320	-0.582049
H	4.376169	-4.076158	0.126062
H	5.554545	-1.942036	0.587607
H	4.346024	0.211346	0.336356
H	1.975950	0.228928	-0.369536
H	-0.118755	-1.906624	1.084790
H	0.224709	-1.137115	-1.712367

PhHC=NPh

Sum of electronic and thermal Free Energies= -556.723247 Hartree/Particle

N	-0.455238	-0.496787	0.118002
C	0.400451	0.403061	-0.174834
C	1.848931	0.181352	-0.084510
C	2.376248	-1.040286	0.361999
C	2.726625	1.209469	-0.451410
C	3.749787	-1.222272	0.436174
H	1.687791	-1.827704	0.642692
C	4.104279	1.025348	-0.375269
H	2.324422	2.156330	-0.797818
C	4.617965	-0.190782	0.068495
H	4.150835	-2.168544	0.781630
H	4.774822	1.827554	-0.661608
H	5.690591	-0.337174	0.128854
H	0.094229	1.397907	-0.527822
C	-1.830850	-0.213500	0.068494
C	-2.383513	0.995186	0.520197
C	-2.688686	-1.216060	-0.406539
C	-3.759106	1.201006	0.466661
H	-1.737016	1.754368	0.945426
C	-4.058953	-0.996422	-0.474684
H	-2.254144	-2.155547	-0.726538
C	-4.601424	0.212972	-0.038865

H	-4.174707	2.134567	0.829912
H	-4.708495	-1.775297	-0.858473
H	-5.672194	0.376614	-0.077719

$PhSiH_3$

Sum of electronic and thermal Free Energies= -522.944530 Hartree/Particle

Si	-2.347260	0.000003	0.006600
H	-2.859532	1.213998	-0.681026
C	-0.465832	0.000019	-0.014367
C	0.257206	1.203115	-0.010885
C	0.257177	-1.203097	-0.010886
C	1.650177	1.205192	0.003423
H	-0.269994	2.152130	-0.024851
C	1.650149	-1.205209	0.003422
H	-0.270043	-2.152100	-0.024857
C	2.349051	-0.000017	0.011668
H	2.189396	2.146141	0.004296
H	2.189342	-2.146173	0.004294
H	3.433390	-0.000027	0.020457
H	-2.859512	-1.213873	-0.681253
H	-2.878972	-0.000155	1.396274

$B(C_6F_5)_3$

Sum of electronic and thermal Free Energies= -2208.767110 Hartree/Particle

C	-0.303654	2.467667	0.753208
C	-0.750395	1.375996	-0.000198
C	-1.910227	1.590392	-0.753581
C	-2.581043	2.803783	-0.774231
C	-2.104649	3.856215	-0.000225
C	-0.961766	3.687996	0.773847
B	0.000472	0.000152	0.000228
C	1.567227	-0.037866	0.000085
C	2.288771	-0.969686	0.755148
C	3.674618	-1.010517	0.776039
C	4.392298	-0.106786	0.000246
C	3.719620	0.830966	-0.775518
C	2.333429	0.857725	-0.754854
F	1.642279	-1.856133	1.528789
F	4.323638	-1.903091	1.527174
F	5.721671	-0.139218	0.000317
F	4.411505	1.690824	-1.526550
F	1.731038	1.774732	-1.528479
F	-2.403588	0.609071	-1.525610
F	-3.673005	2.971646	-1.523596

F	-2.741981	5.023358	-0.000210
F	-0.512652	4.697359	1.523242
F	0.788576	2.352289	1.525320
C	-0.816081	-1.337660	0.000399
C	-1.983981	-1.496705	0.755114
C	-2.712283	-2.676495	0.775527
C	-2.288162	-3.749783	-0.000237
C	-1.139644	-3.635895	-0.775867
C	-0.423445	-2.448784	-0.754769
F	-2.428504	-0.493802	1.528999
F	-3.809949	-2.792502	1.526389
F	-2.980841	-4.884924	-0.000510
F	-0.740746	-4.664853	-1.527022
F	0.671876	-2.385215	-1.528467

H_2O

Sum of electronic and thermal Free Energies= -76.444443 Hartree/Particle

O	0.000000	0.118797	0.000000
H	0.756848	-0.475134	0.000000
H	-0.756848	-0.475245	0.000000

$PhSiH_2OH$

Sum of electronic and thermal Free Energies= -598.232857 Hartree/Particle

Si	-1.927295	0.000047	-0.476630
H	-2.313047	1.211695	-1.252616
C	-0.079664	0.000178	-0.212972
C	0.634806	1.204251	-0.111947
C	0.634554	-1.204085	-0.112024
C	2.012133	1.206438	0.093553
H	0.110482	2.151007	-0.196985
C	2.011871	-1.206594	0.093481
H	0.110023	-2.150719	-0.197149
C	2.701576	-0.000151	0.197612
H	2.547521	2.146407	0.170088
H	2.547060	-2.146682	0.169962
H	3.774474	-0.000269	0.355760
H	-2.312680	-1.211704	-1.252626
O	-2.668244	-0.000096	1.017319
H	-3.627403	0.000160	1.051610

$PhH_2C\text{-}NHPh$

Sum of electronic and thermal Free Energies= -557.914955 Hartree/Particle

N	0.643036	-1.529739	0.021765
C	1.663634	-0.579607	0.030017

C	1.472667	0.719231	0.527853
C	2.514171	1.643776	0.492441
C	3.757602	1.307665	-0.034319
C	3.949916	0.018971	-0.534012
C	2.921561	-0.912448	-0.504720
C	-0.524546	-1.422609	0.881124
C	-1.658116	-0.571857	0.322180
C	-1.818641	-0.384687	-1.051364
C	-2.892083	0.354769	-1.543543
C	-3.820541	0.914468	-0.668623
C	-3.665557	0.734808	0.704642
C	-2.589179	-0.000720	1.194417
H	-0.901476	-2.439188	1.034350
H	0.509320	1.014789	0.922468
H	2.342590	2.642005	0.880721
H	4.561636	2.033399	-0.058159
H	4.911055	-0.265264	-0.948775
H	3.084257	-1.911991	-0.897420
H	-1.087706	-0.812540	-1.727179
H	-3.001149	0.496412	-2.613255
H	-4.654239	1.491646	-1.052460
H	-4.378376	1.173003	1.394559
H	-2.469515	-0.129772	2.266331
H	0.967142	-2.472047	-0.125761
H	-0.250117	-1.042844	1.875663

A-TS1

Sum of electronic and thermal Free Energies= -2808.091940 Hartree/Particle

C	-0.983526	2.447510	0.974441
C	-1.271281	1.449796	0.050079
C	-2.342413	1.735275	-0.795490
C	-3.068191	2.918333	-0.746379
C	-2.732313	3.884900	0.193314
C	-1.678891	3.647874	1.063232
B	-0.467357	0.026644	0.022907
C	-1.510695	-1.234723	0.147280
C	-1.915898	-2.054510	-0.903874
C	-2.803339	-3.115212	-0.750107
C	-3.330916	-3.391738	0.503328
C	-2.962659	-2.600854	1.582958
C	-2.076140	-1.551718	1.379952
F	-1.451426	-1.847074	-2.151531
F	-3.155192	-3.874073	-1.798286
F	-4.183772	-4.411088	0.671318

F	-3.460367	-2.860252	2.804463
F	-1.760107	-0.817869	2.481425
F	-2.714690	0.838280	-1.727918
F	-4.085869	3.140721	-1.590445
F	-3.418361	5.033478	0.258736
F	-1.345922	4.572282	1.981084
F	0.025539	2.290968	1.878002
C	0.637252	-0.162280	-1.171116
C	0.775029	0.570076	-2.348449
C	1.808211	0.364136	-3.259222
C	2.769788	-0.606714	-3.012285
C	2.679895	-1.362409	-1.852203
C	1.624491	-1.120830	-0.988928
F	3.612191	-2.290264	-1.570823
F	3.773986	-0.806737	-3.875734
F	1.890227	1.099758	-4.375996
F	-0.103299	1.538088	-2.665768
F	1.601029	-1.902049	0.150210
C	4.428359	-0.627940	1.410727
C	3.245285	-0.045684	1.902483
C	3.112444	1.354665	1.889403
C	4.152128	2.149438	1.416020
C	5.324518	1.561130	0.943785
C	5.461877	0.173875	0.937345
Si	1.924158	-1.139072	2.575714
O	2.603120	-1.046194	4.474574
H	0.204931	0.002749	1.032955
H	4.535537	-1.706715	1.375346
H	6.364488	-0.283139	0.549523
H	6.126835	2.184210	0.565463
H	4.037991	3.226837	1.397440
H	2.188647	1.820497	2.209579
H	3.329009	-0.424775	4.628543
H	1.980235	-1.006036	5.213636
H	2.134425	-2.586044	2.467040
H	0.597715	-0.676129	2.972959

A-IM1

Sum of electronic and thermal Free Energies= -2808.095110 Hartree/Particle

C	-1.219509	-2.317782	-1.280766
C	-1.483107	-1.350114	-0.316477
C	-2.667597	-1.547194	0.391494
C	-3.534629	-2.608071	0.164385
C	-3.225589	-3.542086	-0.815922

C	-2.054860	-3.397250	-1.544764
B	-0.497490	-0.063831	-0.095730
C	-1.341034	1.343308	-0.039641
C	-1.717161	2.010723	1.124562
C	-2.428179	3.206081	1.129409
C	-2.795547	3.788969	-0.075699
C	-2.443382	3.165577	-1.264362
C	-1.737539	1.969879	-1.218767
F	-1.394453	1.507454	2.332587
F	-2.761937	3.803590	2.282558
F	-3.476404	4.942460	-0.092194
F	-2.779433	3.725417	-2.439855
F	-1.416847	1.425265	-2.422707
F	-3.013960	-0.689842	1.371939
F	-4.660320	-2.745768	0.880241
F	-4.046374	-4.573986	-1.051553
F	-1.741325	-4.296232	-2.493378
F	-0.091235	-2.256124	-2.038733
C	0.575620	-0.199630	1.146520
C	0.587021	-1.159456	2.159763
C	1.588054	-1.244307	3.124714
C	2.647959	-0.346157	3.115346
C	2.684666	0.634387	2.134889
C	1.653728	0.663423	1.213027
F	3.699653	1.511527	2.077501
F	3.619458	-0.426482	4.031485
F	1.543951	-2.192080	4.067867
F	-0.394059	-2.072349	2.253815
F	1.755086	1.708767	0.271443
C	4.759820	0.352868	-1.300862
C	3.415479	0.254019	-1.704941
C	2.888119	-1.009118	-2.027761
C	3.693952	-2.141834	-1.956838
C	5.026227	-2.029692	-1.562406
C	5.559070	-0.784286	-1.232349
Si	2.395419	1.788004	-1.819169
O	2.818825	2.082829	-3.794789
H	0.197039	0.000877	-1.080777
H	5.180251	1.313891	-1.022758
H	6.590996	-0.700469	-0.912237
H	5.647878	-2.915647	-1.500420
H	3.272375	-3.111607	-2.193092
H	1.844612	-1.117198	-2.296953
H	3.382694	1.408976	-4.200164

H	2.087274	2.283114	-4.395179
H	3.059768	3.030669	-1.409426
H	0.972403	1.813771	-2.138125

A-IM2

Sum of electronic and thermal Free Energies= -3364.862984 Hartree/Particle

C	-1.905879	-1.512331	1.995286
C	-2.095594	-1.425896	0.618017
C	-2.635472	-2.572682	0.037223
C	-2.952291	-3.725395	0.747780
C	-2.727945	-3.763960	2.116730
C	-2.205534	-2.644103	2.744020
B	-1.615808	-0.088148	-0.207491
C	-0.818689	-0.499646	-1.588358
C	-1.363998	-0.544106	-2.870818
C	-0.636998	-0.890428	-4.006592
C	0.706006	-1.221949	-3.889182
C	1.292358	-1.197236	-2.633319
C	0.529320	-0.836308	-1.532564
F	-2.661665	-0.254173	-3.069000
F	-1.217519	-0.915087	-5.215555
F	1.424999	-1.563153	-4.969148
F	2.602719	-1.516555	-2.492888
F	1.197474	-0.827287	-0.340157
F	-2.876563	-2.611704	-1.287215
F	-3.461073	-4.803210	0.128956
F	-2.998820	-4.872801	2.824328
F	-1.949498	-2.683275	4.071765
F	-1.375003	-0.477980	2.691866
C	-2.785231	1.039214	-0.431849
C	-4.156055	0.803816	-0.513483
C	-5.104699	1.812990	-0.645265
C	-4.694578	3.137134	-0.708907
C	-3.339644	3.426297	-0.639443
C	-2.432173	2.384463	-0.506560
F	-2.921101	4.704938	-0.697822
F	-5.594073	4.123347	-0.837597
F	-6.413423	1.521862	-0.716229
F	-4.638355	-0.454619	-0.473169
F	-1.122181	2.752639	-0.446377
C	0.988655	5.009702	1.153587
C	1.760313	4.015649	1.778651
C	2.564261	4.385306	2.869747
C	2.608441	5.704419	3.314288

C	1.838448	6.677126	2.679586
C	1.025681	6.327536	1.603043
Si	1.662077	2.245712	1.177804
O	3.201958	1.513691	1.431540
H	-0.793814	0.438970	0.486754
H	0.342145	4.751261	0.321345
H	0.418445	7.080097	1.112974
H	1.867673	7.703865	3.026970
H	3.235514	5.971826	4.157637
H	3.156947	3.637699	3.390152
H	3.935041	2.134068	1.496543
H	3.706135	-0.072346	0.806122
H	1.393041	2.219278	-0.272302
H	0.746635	1.396821	1.957038
N	4.192053	-0.866734	0.342670
C	3.882940	-2.098675	0.626665
C	2.959806	-2.550856	1.625078
C	2.272105	-1.686916	2.503439
C	2.710252	-3.938063	1.679031
C	1.341638	-2.203832	3.386534
H	2.452766	-0.619914	2.482358
C	1.782334	-4.447678	2.573428
H	3.235115	-4.603409	1.002173
C	1.091283	-3.580028	3.419093
H	0.780136	-1.539961	4.030287
H	1.581525	-5.511386	2.601866
H	0.337077	-3.965452	4.094358
H	4.372749	-2.855453	0.021630
C	5.151865	-0.480293	-0.641754
C	6.334777	-1.200761	-0.812949
C	4.879416	0.646223	-1.419889
C	7.238100	-0.801930	-1.792854
H	6.564648	-2.042313	-0.170127
C	5.792707	1.036338	-2.392471
H	3.949248	1.182111	-1.283064
C	6.969315	0.313539	-2.583559
H	8.159420	-1.355752	-1.926872
H	5.577597	1.900256	-3.009422
H	7.677185	0.621564	-3.343532

A-IM3

Sum of electronic and thermal Free Energies= -2766.645687 Hartree/Particle

C	1.909049	-3.415227	0.872280
N	2.039100	-2.123540	0.928158

C	3.294651	-1.440263	0.816481
C	3.546707	-0.359075	1.661551
C	4.766940	0.300062	1.561412
C	5.714713	-0.107782	0.623635
C	5.440903	-1.176088	-0.227991
C	4.225734	-1.846557	-0.139818
F	0.522621	-0.161858	2.606095
C	-0.342998	0.899790	2.504851
C	-0.860644	1.265671	1.269916
C	-1.736022	2.350259	1.314678
C	-2.066850	3.021515	2.485700
C	-1.511239	2.612377	3.691663
C	-0.635223	1.537297	3.703073
B	-0.498874	0.434579	-0.095371
C	0.764160	1.040263	-0.949140
C	1.565257	0.182633	-1.699157
C	2.683148	0.583980	-2.416719
C	3.041899	1.923484	-2.417145
C	2.270281	2.826853	-1.700134
C	1.161935	2.375542	-0.990348
F	-2.302728	2.805492	0.182953
F	-2.911692	4.061272	2.467752
F	-1.814914	3.249677	4.829131
F	-0.084710	1.126709	4.857981
F	1.286935	-1.149726	-1.739929
F	3.432684	-0.313148	-3.084397
F	4.121116	2.336812	-3.095101
F	2.604960	4.125425	-1.696346
F	0.464982	3.319964	-0.329864
C	-1.839658	0.138606	-0.992845
C	-2.807501	-0.735554	-0.506846
C	-3.953366	-1.099864	-1.197954
C	-4.185248	-0.554105	-2.452728
C	-3.263186	0.339245	-2.979483
C	-2.123920	0.667276	-2.249858
F	-2.649246	-1.303258	0.721868
F	-1.286316	1.548852	-2.831049
F	-3.480719	0.877649	-4.188024
F	-5.283084	-0.886091	-3.144255
F	-4.827567	-1.976321	-0.670628
H	-0.131349	-0.666333	0.278338
H	2.801351	-0.052204	2.383000
H	4.973201	1.138544	2.215276
H	6.657722	0.419365	0.543050

H	6.158238	-1.469951	-0.984149
H	3.979592	-2.630422	-0.845264
H	1.202521	-1.522490	0.990056
H	2.839889	-3.971273	0.808788
C	0.688752	-4.172386	0.896798
C	0.805543	-5.577865	0.863855
C	-0.589740	-3.581818	0.940939
C	-0.329893	-6.372530	0.874938
H	1.788452	-6.035002	0.826709
C	-1.719118	-4.383907	0.943933
H	-0.709681	-2.506567	0.957103
C	-1.591120	-5.775145	0.912547
H	-0.237762	-7.451322	0.849434
H	-2.696221	-3.917956	0.959232
H	-2.479845	-6.395670	0.914009

A-TS2

Sum of electronic and thermal Free Energies= -2766.635646 Hartree/Particle

C	0.286318	-0.862042	2.339817
N	1.232689	-0.094406	2.898237
C	2.610476	-0.084189	2.554632
C	3.284106	1.139589	2.540021
C	4.640772	1.176703	2.235377
C	5.327212	0.001481	1.939200
C	4.650730	-1.217432	1.961283
C	3.297371	-1.268674	2.277167
F	0.135196	2.186555	1.812237
C	-0.080399	2.600996	0.530365
C	-0.203880	1.679827	-0.497986
C	-0.435149	2.241212	-1.754468
C	-0.524399	3.606591	-1.983442
C	-0.386749	4.485345	-0.915245
C	-0.159905	3.977178	0.354436
B	-0.172366	0.056325	-0.353195
C	1.149151	-0.704399	-0.917485
C	1.285118	-2.085168	-0.765157
C	2.388255	-2.817217	-1.169910
C	3.448814	-2.154825	-1.774771
C	3.375962	-0.781747	-1.948129
C	2.248275	-0.087610	-1.517603
F	-0.555824	1.433025	-2.825779
F	-0.736040	4.086429	-3.214850
F	-0.467915	5.805381	-1.110791
F	-0.022110	4.809327	1.398386

F	0.296325	-2.791449	-0.150463
F	2.450337	-4.141564	-0.970939
F	4.531713	-2.832507	-2.168176
F	4.397360	-0.131088	-2.518918
F	2.282369	1.243923	-1.710004
C	-1.618759	-0.555021	-0.777702
C	-2.760438	-0.169798	-0.072899
C	-4.042180	-0.608398	-0.373680
C	-4.227475	-1.466530	-1.448753
C	-3.128745	-1.863294	-2.198468
C	-1.860877	-1.404824	-1.858031
F	-2.647070	0.680271	0.971421
F	-0.854674	-1.815977	-2.651494
F	-3.301677	-2.679765	-3.246092
F	-5.451805	-1.904693	-1.759528
F	-5.093985	-0.217468	0.360580
H	-0.098982	-0.196228	0.947422
H	2.739525	2.055704	2.738620
H	5.156928	2.129105	2.217585
H	6.382071	0.033243	1.695201
H	5.180511	-2.137149	1.743362
H	2.789870	-2.224297	2.326426
H	0.915399	0.728991	3.390060
H	0.652701	-1.734420	1.817159
C	-1.048027	-0.990515	2.942436
C	-1.803561	-2.124677	2.613051
C	-1.584001	-0.039616	3.822282
C	-3.065943	-2.311257	3.165296
H	-1.398997	-2.852598	1.919562
C	-2.845238	-0.228260	4.367617
H	-1.040220	0.865609	4.065462
C	-3.588619	-1.363768	4.041514
H	-3.642181	-3.191455	2.906800
H	-3.256535	0.514485	5.040509
H	-4.576140	-1.503360	4.465240

B-TS1

Sum of electronic and thermal Free Energies= -3288.388570 Hartree/Particle

C	1.515469	-1.684085	2.020147
C	2.052665	-0.514447	1.489326
C	3.028528	0.091883	2.279386
C	3.427823	-0.409542	3.513590
C	2.843736	-1.568594	4.004858
C	1.874162	-2.215022	3.249603

B	1.584869	0.058693	0.051142
C	1.966743	-0.821516	-1.247226
C	2.936401	-1.821976	-1.276269
C	3.214758	-2.574084	-2.413282
C	2.507700	-2.338138	-3.583527
C	1.536329	-1.345306	-3.605543
C	1.301621	-0.611925	-2.454155
F	3.674928	-2.100871	-0.185468
F	4.158743	-3.523127	-2.388426
F	2.758943	-3.058146	-4.680583
F	0.843982	-1.108397	-4.727745
F	0.359033	0.356772	-2.530449
F	3.659308	1.205179	1.858772
F	4.371948	0.212739	4.229524
F	3.212787	-2.060569	5.190622
F	1.304254	-3.337541	3.708083
F	0.583621	-2.368461	1.314425
C	1.701681	1.666311	-0.108295
C	0.960653	2.526760	0.696979
C	1.029044	3.908955	0.621141
C	1.888442	4.495293	-0.297287
C	2.665948	3.683118	-1.110833
C	2.561941	2.300207	-1.003924
F	0.107833	2.014092	1.620573
F	0.266478	4.681278	1.414316
F	1.967154	5.825457	-0.392898
F	3.508832	4.237918	-1.989250
F	3.367248	1.582001	-1.806882
H	0.227197	-0.151465	0.075583
Si	-1.416754	-0.153336	0.208280
N	-3.915330	0.177137	0.773307
C	-1.884253	-1.563310	-0.914227
C	-1.861877	-2.900557	-0.487434
C	-2.211619	-3.928698	-1.357998
C	-2.586706	-3.638988	-2.668373
C	-2.613935	-2.316863	-3.108280
C	-2.267034	-1.287366	-2.237680
H	-1.566820	-3.143496	0.525457
H	-2.188077	-4.956261	-1.013554
H	-2.852430	-4.441857	-3.347075
H	-2.894839	-2.087861	-4.129969
H	-2.280097	-0.264898	-2.598089
C	-4.725132	1.103029	0.409589
C	-4.477225	-1.081663	1.138852

C	-5.340219	-1.781576	0.289531
C	-5.852635	-3.014862	0.681916
C	-5.511750	-3.557800	1.918634
C	-4.644617	-2.863920	2.761213
C	-4.118213	-1.636247	2.371567
H	-5.576334	-1.376740	-0.687568
H	-6.511831	-3.556381	0.013140
H	-5.911943	-4.518469	2.220805
H	-4.374091	-3.279608	3.725062
H	-3.447414	-1.090093	3.023308
H	-1.592872	1.179681	-0.374342
H	-1.406474	-0.371063	1.659095
H	-5.797616	0.882363	0.359335
C	-4.365305	2.481694	0.069458
C	-3.219442	3.116860	0.573358
C	-5.245098	3.210329	-0.746416
C	-2.948124	4.438197	0.239281
H	-2.561572	2.586004	1.247966
C	-4.962590	4.526264	-1.092962
H	-6.147521	2.735215	-1.117132
C	-3.812074	5.140756	-0.601575
H	-2.064299	4.919370	0.639529
H	-5.641426	5.074400	-1.735687
H	-3.594640	6.170507	-0.861033

B-IM1

Sum of electronic and thermal Free Energies= -3288.388735 Hartree/Particle

C	-1.621763	-1.412880	-2.268152
C	-2.164162	-0.475860	-1.396096
C	-3.417858	0.004714	-1.773108
C	-4.076098	-0.387619	-2.931973
C	-3.478433	-1.313022	-3.776710
C	-2.238128	-1.833914	-3.439478
B	-1.411614	0.024267	-0.035345
C	-1.709579	-0.858248	1.302162
C	-2.623916	-1.904097	1.406274
C	-2.788026	-2.663325	2.561915
C	-2.013662	-2.392252	3.679472
C	-1.090315	-1.356954	3.626888
C	-0.971358	-0.620369	2.459829
F	-3.417357	-2.241225	0.369345
F	-3.684951	-3.659445	2.602341
F	-2.149527	-3.122156	4.793820
F	-0.317049	-1.091648	4.692832

F	-0.057221	0.382189	2.472498
F	-4.073962	0.878875	-0.983210
F	-5.281147	0.111368	-3.240161
F	-4.093958	-1.702720	-4.899444
F	-1.649452	-2.736263	-4.240859
F	-0.421120	-1.987276	-1.995927
C	-1.558936	1.643456	0.161244
C	-0.879532	2.525114	-0.672584
C	-0.961595	3.906741	-0.577672
C	-1.765460	4.474326	0.398652
C	-2.480953	3.641287	1.247271
C	-2.369346	2.261223	1.113220
F	-0.064109	2.044652	-1.651964
F	-0.248494	4.698701	-1.405220
F	-1.848229	5.805209	0.518211
F	-3.272755	4.176508	2.185867
F	-3.115178	1.526668	1.957277
H	-0.171291	-0.167281	-0.238246
Si	1.733188	-0.139200	-0.388697
N	3.737339	0.102977	-0.791582
C	1.919794	-1.675692	0.654820
C	1.667820	-2.964487	0.160718
C	1.828226	-4.080296	0.977983
C	2.238027	-3.927605	2.301040
C	2.485430	-2.653931	2.809117
C	2.328251	-1.537633	1.991694
H	1.331412	-3.099789	-0.859161
H	1.623082	-5.069056	0.583569
H	2.352168	-4.797471	2.938195
H	2.781599	-2.527239	3.844152
H	2.496559	-0.551826	2.411772
C	4.529088	1.092481	-0.531888
C	4.370731	-1.112744	-1.260484
C	5.242845	-1.824108	-0.437141
C	5.834851	-2.990759	-0.912098
C	5.555005	-3.446683	-2.198492
C	4.677277	-2.733746	-3.012000
C	4.076678	-1.566947	-2.545692
H	5.426840	-1.484838	0.575203
H	6.505118	-3.549233	-0.269498
H	6.014535	-4.357537	-2.563402
H	4.456790	-3.082683	-4.013829
H	3.397919	-1.006248	-3.175778
H	1.637647	1.116653	0.357338

H	1.424272	-0.244036	-1.817020
H	5.598634	0.888126	-0.613887
Si	4.203353	2.462394	-0.158937
Si	3.047594	3.141876	-0.581751
Si	5.167075	3.154710	0.598043
Si	2.850651	4.468506	-0.219477
H	2.322300	2.656104	-1.219694
C	4.950905	4.470621	0.981278
H	6.078443	2.647745	0.896900
C	3.790595	5.127675	0.572790
H	1.962458	4.984752	-0.560367
H	5.688556	4.987550	1.583125
H	3.625138	6.160272	0.857472

B-IM2

Sum of electronic and thermal Free Energies= -3288.392548 Hartree/Particle

C	-1.866131	2.502878	0.618957
C	-1.543175	1.460522	-0.248657
C	-0.908549	1.866620	-1.418798
C	-0.589525	3.183356	-1.721333
C	-0.920936	4.180123	-0.816999
C	-1.566458	3.837094	0.362420
B	-1.810350	-0.137975	0.034322
C	-1.678095	-0.533565	1.624161
C	-0.416626	-0.650729	2.196807
C	-0.173370	-1.018181	3.511434
C	-1.248966	-1.301627	4.339782
C	-2.534856	-1.199369	3.826656
C	-2.723853	-0.819198	2.500785
F	0.701302	-0.385404	1.449739
F	1.087632	-1.103008	3.983325
F	-1.048897	-1.662307	5.614748
F	-3.583033	-1.463500	4.620083
F	-4.003393	-0.727375	2.093999
F	-0.521056	0.943121	-2.347540
F	0.066370	3.497349	-2.853826
F	-0.589284	5.457448	-1.065821
F	-1.878663	4.797402	1.247479
F	-2.496327	2.252235	1.781877
C	-3.177769	-0.675685	-0.693050
C	-3.210298	-1.912182	-1.331217
C	-4.316120	-2.409763	-2.009573
C	-5.474468	-1.649362	-2.065314
C	-5.500774	-0.410168	-1.439757

C	-4.368581	0.044207	-0.774026
F	-2.115793	-2.720640	-1.324722
F	-4.474646	1.247478	-0.175534
F	-6.619192	0.330140	-1.483190
F	-6.555108	-2.106036	-2.713331
F	-4.272806	-3.611664	-2.612237
H	-0.895636	-0.712052	-0.499692
C	2.130414	-0.566025	-1.239881
N	2.918804	0.059244	-0.399730
Si	3.953955	-0.697841	0.946955
C	2.864340	1.518245	-0.433155
C	2.331395	2.235267	0.637482
C	2.275713	3.623272	0.556743
C	2.745533	4.286511	-0.576140
C	3.275970	3.559905	-1.638242
C	3.341628	2.170280	-1.570039
H	1.923931	1.713204	1.491562
H	1.839166	4.185297	1.373349
H	2.678734	5.365731	-0.636837
H	3.627710	4.068911	-2.527119
H	3.757876	1.595631	-2.389134
C	5.743055	-0.801848	0.425913
C	6.407494	-2.039411	0.457854
C	7.758612	-2.133829	0.131320
C	8.465974	-0.992192	-0.236687
C	7.823991	0.245071	-0.270711
C	6.476451	0.341269	0.062454
H	5.870868	-2.938079	0.745945
H	8.257253	-3.095616	0.166568
H	9.516994	-1.064363	-0.492038
H	8.375356	1.135285	-0.550775
H	5.998265	1.315000	0.042006
H	1.384807	0.052729	-1.735072
C	2.130340	-1.967784	-1.585957
C	0.902631	-2.516187	-2.004770
C	3.287127	-2.772438	-1.585241
C	0.820493	-3.859449	-2.343716
H	0.013164	-1.900159	-2.006599
C	3.201748	-4.103022	-1.963499
H	4.253815	-2.344590	-1.351413
C	1.967641	-4.651043	-2.325798
H	-0.138644	-4.278171	-2.621011
H	4.095337	-4.715104	-1.986715
H	1.906638	-5.695949	-2.607824

H	3.748431	0.250720	2.052445
H	3.384743	-2.030012	1.204783

$PhHC=N^{+}Ph(SiH_2Ph)$

Sum of electronic and thermal Free Energies= -1078.850193 Hartree/Particle

C	0.601556	-1.689230	-0.133333
N	-0.349357	-0.948015	0.379223
Si	-0.208726	0.548979	1.501276
C	-1.715613	-1.385133	0.088799
C	-2.496482	-1.960485	1.090192
C	-3.786716	-2.381365	0.781319
C	-4.291104	-2.218816	-0.508626
C	-3.502663	-1.639407	-1.499346
C	-2.206779	-1.218835	-1.205654
H	-2.100409	-2.094338	2.089245
H	-4.395907	-2.840678	1.550111
H	-5.297508	-2.545583	-0.740084
H	-3.891163	-1.512875	-2.502503
H	-1.589669	-0.755708	-1.966685
C	-0.299610	2.134608	0.543490
C	0.769365	3.046502	0.601635
C	0.693646	4.273025	-0.053531
C	-0.449072	4.604626	-0.777360
C	-1.521431	3.715057	-0.839243
C	-1.451818	2.492267	-0.180349
H	1.661417	2.810623	1.173716
H	1.521266	4.969819	0.006351
H	-0.508843	5.559459	-1.286341
H	-2.414497	3.979810	-1.392849
H	-2.304144	1.822430	-0.224641
H	0.258680	-2.624829	-0.573037
C	2.022995	-1.464588	-0.192526
C	2.829985	-2.614931	-0.332951
C	2.633623	-0.193759	-0.176690
C	4.210281	-2.501330	-0.383646
H	2.365748	-3.593648	-0.382111
C	4.012525	-0.088046	-0.258970
H	2.032662	0.705539	-0.168810
C	4.801842	-1.238161	-0.344590
H	4.824516	-3.388817	-0.469679
H	4.478314	0.889541	-0.270707
H	5.879984	-1.146532	-0.403248
H	-1.362142	0.312494	2.385555
H	1.082183	0.371704	2.191575

$(C_6F_5)_3B\text{-}H^-$

Sum of electronic and thermal Free Energies= -2209.472452 Hartree/Particle

H	0.001497	0.000888	1.993276
B	0.000783	0.000253	0.789460
C	1.478813	0.563944	0.345394
C	2.596595	0.241980	1.114515
C	1.745188	1.391696	-0.742104
C	3.878258	0.709445	0.847711
C	3.009422	1.886132	-1.043844
C	4.086503	1.542910	-0.241145
C	-0.249632	-1.561946	0.346412
C	-1.083964	-2.370580	1.117453
C	0.329616	-2.204073	-0.744904
C	-1.321034	-3.713763	0.848647
C	0.124488	-3.545379	-1.048750
C	-0.707552	-4.308445	-0.243793
C	-1.227234	0.997715	0.345967
C	-1.512628	2.122895	1.118604
C	-2.072705	0.817107	-0.745685
C	-2.558554	2.998553	0.850740
C	-3.132892	1.664426	-1.048727
C	-3.379438	2.765155	-0.242407
F	2.475879	-0.568986	2.187588
F	4.920842	0.367560	1.631463
F	5.319344	2.008057	-0.518248
F	3.205284	2.687129	-2.110253
F	0.757497	1.753304	-1.590991
F	-2.788614	4.069070	1.637670
F	-0.755115	2.421424	2.195954
F	-4.398742	3.599892	-0.520419
F	-3.919567	1.437128	-2.119534
F	-1.885931	-0.214945	-1.598231
F	1.132296	-1.527174	-1.595880
F	-1.723029	-1.862639	2.193161
F	0.715147	-4.113233	-2.119181
F	-0.922175	-5.608101	-0.522868
F	-2.135885	-4.447237	1.633650

B-TS2

Sum of electronic and thermal Free Energies= -3288.382749 Hartree/Particle

C	-1.743079	2.759193	0.338833
C	-1.237342	1.707631	-0.427369
C	-0.608811	2.115436	-1.604817

C	-0.464594	3.432283	-2.003799
C	-0.982152	4.439881	-1.201089
C	-1.630189	4.098694	-0.025867
B	-1.323177	0.131702	-0.018787
C	-1.834674	-0.159805	1.499592
C	-0.999981	-0.236544	2.604802
C	-1.437513	-0.490601	3.897762
C	-2.793169	-0.672794	4.126615
C	-3.677581	-0.592047	3.058306
C	-3.188674	-0.340752	1.783229
F	0.343781	-0.063971	2.456453
F	-0.566227	-0.565203	4.915565
F	-3.243714	-0.919188	5.361132
F	-4.989738	-0.751374	3.271021
F	-4.102165	-0.240575	0.797753
F	-0.084670	1.183287	-2.443338
F	0.181732	3.744899	-3.135838
F	-0.834451	5.722529	-1.549462
F	-2.127902	5.061866	0.762023
F	-2.385174	2.534907	1.502060
C	-2.021990	-0.869794	-1.096831
C	-2.013486	-2.248585	-0.870039
C	-2.580486	-3.184347	-1.723250
C	-3.224594	-2.749195	-2.872617
C	-3.291443	-1.388922	-3.134365
C	-2.706385	-0.485897	-2.252891
F	-1.440212	-2.742183	0.249304
F	-2.866633	0.812788	-2.570141
F	-3.929061	-0.955254	-4.229920
F	-3.779325	-3.629281	-3.712059
F	-2.519088	-4.494584	-1.445444
H	-0.027337	-0.254434	-0.013233
C	1.495791	-0.496401	-0.421628
N	2.305796	0.225357	0.383218
Si	3.488207	-0.357987	1.647112
C	2.443782	1.636645	0.066160
C	1.986095	2.597374	0.968357
C	2.136621	3.947958	0.667593
C	2.738440	4.340713	-0.527240
C	3.195947	3.377833	-1.423203
C	3.058699	2.024040	-1.125237
H	1.502095	2.282210	1.883907
H	1.770978	4.694036	1.363292
H	2.841627	5.393406	-0.762104

H	3.660469	3.676899	-2.355069
H	3.428132	1.270264	-1.810533
C	5.092062	-0.856184	0.825952
C	5.306934	-2.170167	0.375877
C	6.508599	-2.529446	-0.228366
C	7.517705	-1.582268	-0.393154
C	7.324602	-0.275421	0.049485
C	6.122544	0.083586	0.654244
H	4.533614	-2.921071	0.499289
H	6.658984	-3.548228	-0.567361
H	8.454358	-1.863482	-0.861388
H	8.110314	0.461733	-0.071739
H	5.990225	1.103412	1.000825
H	1.263706	-0.016429	-1.363705
C	1.543972	-1.976922	-0.493472
C	1.761203	-2.536428	-1.760748
C	1.387699	-2.825755	0.608687
C	1.872959	-3.914645	-1.914448
H	1.849945	-1.888698	-2.625802
C	1.489482	-4.202579	0.449979
H	1.136788	-2.412862	1.574765
C	1.742176	-4.749741	-0.807400
H	2.047557	-4.334139	-2.898124
H	1.344696	-4.851347	1.305515
H	1.812210	-5.824665	-0.927014
H	3.699663	0.832400	2.491898
H	2.912991	-1.467277	2.420601

B-IM3

Sum of electronic and thermal Free Energies= -3288.428895 Hartree/Particle

C	2.302931	-3.013860	-0.248150
C	2.258900	-1.661799	-0.617002
C	2.044160	-1.414074	-1.980231
C	1.866215	-2.424382	-2.911484
C	1.921852	-3.749567	-2.495900
C	2.150383	-4.048818	-1.157136
B	2.418054	-0.507815	0.423449
C	1.876444	-0.666348	1.887674
C	0.627089	-1.230267	2.165055
C	0.121582	-1.340630	3.451163
C	0.888854	-0.899115	4.523975
C	2.144361	-0.346013	4.298060
C	2.607665	-0.227557	2.995845
F	-0.156742	-1.652363	1.160588

F	-1.091966	-1.854211	3.669850
F	0.422182	-1.006515	5.764839
F	2.884528	0.066462	5.329855
F	3.828412	0.307088	2.827000
F	1.963523	-0.154448	-2.435700
F	1.636407	-2.140846	-4.195520
F	1.760097	-4.730381	-3.377647
F	2.218232	-5.322773	-0.764069
F	2.531746	-3.359565	1.027866
C	3.104703	0.844500	0.016159
C	2.571691	2.081779	0.386314
C	3.144570	3.290445	0.021881
C	4.322187	3.286465	-0.717077
C	4.900283	2.078615	-1.093923
C	4.282308	0.889864	-0.735603
F	1.424676	2.139080	1.090427
F	4.876087	-0.251136	-1.119799
F	6.035392	2.077306	-1.796053
F	4.893971	4.435726	-1.065381
F	2.576883	4.449355	0.368415
H	-2.211922	1.721029	1.307333
C	-2.051556	1.519666	0.245355
N	-2.838178	0.332564	-0.100753
Si	-3.819972	-0.438801	1.150995
C	-2.581537	-0.295036	-1.338046
C	-3.368370	-1.385063	-1.758994
C	-3.107136	-2.043834	-2.953746
C	-2.064008	-1.633800	-3.781837
C	-1.296090	-0.541032	-3.391781
C	-1.546389	0.124240	-2.193938
H	-4.208506	-1.713188	-1.159320
H	-3.735101	-2.879976	-3.241623
H	-1.863305	-2.145107	-4.715671
H	-0.488861	-0.191607	-4.025231
H	-0.938633	0.981597	-1.943662
C	-5.679243	-0.400446	0.860539
C	-6.371716	0.806302	0.666625
C	-7.753476	0.822570	0.497864
C	-8.473936	-0.370975	0.522331
C	-7.807713	-1.578050	0.716997
C	-6.423722	-1.589735	0.883659
H	-5.829817	1.746722	0.647750
H	-8.269197	1.764918	0.349063
H	-9.550271	-0.358723	0.390969

H	-8.363639	-2.508978	0.737773
H	-5.918342	-2.539241	1.033473
H	-0.980201	1.307365	0.146958
C	-2.375009	2.794104	-0.526052
C	-3.553367	2.947242	-1.257007
C	-1.476420	3.865388	-0.465020
C	-3.833180	4.149232	-1.906677
H	-4.245697	2.117727	-1.330705
C	-1.756398	5.066906	-1.109366
H	-0.549695	3.758330	0.090856
C	-2.939082	5.213579	-1.833026
H	-4.750704	4.249304	-2.476159
H	-1.048863	5.886674	-1.050319
H	-3.156857	6.147001	-2.339690
H	-3.436450	-1.864766	1.306006
H	-3.495195	0.327294	2.379248

PhH_2C-$NPhSiH_2Ph$

Sum of electronic and thermal Free Energies= -1079.673560 Hartree/Particle

H	-1.235805	-0.744249	2.413589
C	-1.517634	-0.086284	1.588104
N	-0.299621	0.576595	1.114861
Si	1.257334	0.078983	1.785162
C	-0.440700	1.721722	0.300313
C	0.696701	2.389325	-0.193905
C	0.579247	3.535539	-0.969853
C	-0.672832	4.054689	-1.291515
C	-1.805031	3.393993	-0.826399
C	-1.699702	2.244871	-0.047387
H	1.688237	2.006256	0.013273
H	1.479596	4.021312	-1.329989
H	-0.762376	4.947097	-1.899300
H	-2.792436	3.768305	-1.074358
H	-2.607071	1.752122	0.270621
C	2.470846	-0.677815	0.562081
C	2.146448	-1.822828	-0.184302
C	3.069806	-2.400239	-1.051537
C	4.341187	-1.844539	-1.188798
C	4.684732	-0.712004	-0.455217
C	3.756461	-0.136206	0.410713
H	1.163252	-2.272821	-0.089069
H	2.799563	-3.284054	-1.618952
H	5.060668	-2.294043	-1.864224
H	5.672669	-0.276575	-0.557567

H	4.039634	0.746938	0.975771
H	-2.200200	0.654541	2.023066
C	-2.277384	-0.922582	0.563691
C	-1.750528	-1.239520	-0.688416
C	-3.538956	-1.421468	0.907265
C	-2.466241	-2.043280	-1.576128
H	-0.784078	-0.844465	-0.975356
C	-4.252974	-2.226376	0.025068
H	-3.965703	-1.178247	1.876306
C	-3.716817	-2.541460	-1.223082
H	-2.044522	-2.274044	-2.548270
H	-5.228515	-2.605248	0.309511
H	-4.272589	-3.164978	-1.914249
H	1.949279	1.234085	2.415535
H	0.895284	-0.927079	2.813198

B-IM4

Sum of electronic and thermal Free Energies= -3364.877062 Hartree/Particle

C	-3.070637	-0.532161	-2.175203
C	-2.030447	-0.704197	-1.262953
C	-1.063368	-1.630933	-1.647556
C	-1.075208	-2.317781	-2.851037
C	-2.126417	-2.102687	-3.732643
C	-3.132468	-1.209794	-3.388868
B	-1.906916	0.033634	0.189706
C	-2.040158	-1.080810	1.371959
C	-3.246161	-1.774748	1.483644
C	-3.473621	-2.779083	2.412423
C	-2.452474	-3.147016	3.281137
C	-1.227091	-2.503346	3.198982
C	-1.053139	-1.498674	2.255103
F	-4.263698	-1.459715	0.661114
F	-4.656631	-3.396756	2.478205
F	-2.647189	-4.114611	4.179231
F	-0.224630	-2.856265	4.012202
F	0.195244	-0.939794	2.218876
F	-0.025884	-1.897527	-0.808642
F	-0.093317	-3.171527	-3.167344
F	-2.168391	-2.749165	-4.899484
F	-4.150804	-1.005068	-4.230790
F	-4.084306	0.309765	-1.913543
C	-2.754751	1.412275	0.364442
C	-2.511944	2.459195	-0.523595
C	-3.144651	3.689458	-0.478747

C	-4.085450	3.919206	0.518031
C	-4.355395	2.919771	1.440426
C	-3.687534	1.700052	1.358016
F	-1.586859	2.286234	-1.508252
F	-3.994439	0.803015	2.311651
F	-5.247362	3.138562	2.412535
F	-4.713173	5.094488	0.591821
F	-2.858968	4.647888	-1.367668
O	-0.370412	0.618458	0.259222
C	3.112818	-1.464677	0.406666
N	2.914957	-0.013885	0.234148
Si	3.273054	1.042404	1.623218
C	4.497794	-2.017063	0.095006
C	4.818064	-3.302734	0.547362
C	6.058917	-3.867998	0.272948
C	7.006249	-3.152868	-0.459162
C	6.699174	-1.872980	-0.910355
C	5.452887	-1.308038	-0.635285
C	2.554276	0.473162	-1.039344
C	2.537613	-0.345011	-2.185589
C	2.125784	0.157518	-3.416344
C	1.721971	1.482574	-3.558626
C	1.743896	2.308018	-2.438063
C	2.148909	1.816798	-1.198479
C	4.654635	2.287101	1.373967
C	4.376914	3.662815	1.402687
C	5.393027	4.606265	1.264604
C	6.710541	4.187902	1.097433
C	7.008914	2.826205	1.073301
C	5.991555	1.886217	1.211209
H	3.356102	4.005964	1.541574
H	5.156731	5.664208	1.289067
H	7.503526	4.919644	0.990457
H	8.034926	2.497425	0.950774
H	6.244840	0.831445	1.195554
H	2.871433	-1.711661	1.442794
H	2.859126	-1.374953	-2.128522
H	2.126912	-0.504806	-4.274955
H	1.403707	1.865022	-4.520405
H	1.440995	3.345774	-2.518411
H	2.166421	2.495442	-0.354257
H	4.088997	-3.864347	1.123988
H	6.289336	-4.863775	0.634848
H	7.974674	-3.590461	-0.672985

H	7.427790	-1.308585	-1.481766
H	5.226554	-0.311977	-0.994582
H	0.323894	0.008286	0.559280
H	-0.061739	1.074132	-0.545582
H	2.367826	-1.990988	-0.197382
H	2.056040	1.820837	1.977766
H	3.597848	0.083740	2.702176

B-TS3

Sum of electronic and thermal Free Energies= -3364.871607 Hartree/Particle

C	3.005184	1.037038	1.815082
C	2.056299	1.182500	0.802334
C	1.648619	2.494632	0.585626
C	2.113664	3.582626	1.317715
C	3.049924	3.378608	2.318785
C	3.501145	2.088500	2.571054
B	1.603891	-0.132600	-0.090681
C	0.889927	-1.347880	0.755134
C	0.436775	-1.273504	2.069737
C	-0.178424	-2.327218	2.737793
C	-0.378180	-3.530127	2.078707
C	0.030697	-3.651193	0.757113
C	0.639411	-2.572518	0.130658
F	0.530855	-0.122265	2.777636
F	-0.604853	-2.175849	4.000160
F	-0.976412	-4.551361	2.698398
F	-0.184429	-4.796465	0.096810
F	0.986454	-2.756297	-1.158343
F	0.736316	2.797670	-0.381100
F	1.665663	4.819916	1.060542
F	3.511958	4.408779	3.034486
F	4.403356	1.877045	3.536926
F	3.473047	-0.192890	2.107611
C	2.946766	-0.587680	-0.942320
C	3.360173	0.167313	-2.036528
C	4.491943	-0.095054	-2.793734
C	5.290230	-1.176662	-2.448033
C	4.935057	-1.959289	-1.358728
C	3.787272	-1.655827	-0.633028
F	2.633387	1.263282	-2.413458
F	3.519501	-2.468687	0.405607
F	5.699726	-3.003969	-1.017875
F	6.388524	-1.458686	-3.155861
F	4.819999	0.677196	-3.838167

O	0.519580	0.250089	-1.124916
C	-1.952232	1.376216	0.590437
N	-1.925398	0.658086	-0.743886
Si	-2.680950	-1.038823	-0.759188
C	-3.188715	1.257579	1.462177
C	-3.019886	0.806325	2.778077
C	-4.095738	0.749115	3.660252
C	-5.364186	1.140214	3.239227
C	-5.548112	1.580440	1.930587
C	-4.471283	1.639612	1.049631
C	-2.226581	1.456695	-1.935224
C	-2.872822	2.692036	-1.887479
C	-3.100450	3.408811	-3.061517
C	-2.689904	2.907384	-4.291867
C	-2.032150	1.680885	-4.340660
C	-1.795515	0.961164	-3.173309
C	-4.501264	-1.118047	-1.162103
C	-4.984824	-0.896842	-2.463395
C	-6.338789	-1.036085	-2.754211
C	-7.232527	-1.412706	-1.753083
C	-6.770089	-1.646969	-0.460187
C	-5.417090	-1.497774	-0.166948
H	-4.303351	-0.614705	-3.258366
H	-6.695221	-0.858480	-3.762553
H	-8.286002	-1.528547	-1.982143
H	-7.461296	-1.945279	0.319819
H	-5.074271	-1.675658	0.846490
H	-1.110446	0.976131	1.154535
H	-3.194356	3.116388	-0.947474
H	-3.601278	4.368174	-3.004015
H	-2.868508	3.470121	-5.200123
H	-1.686005	1.283250	-5.287538
H	-1.259507	0.021596	-3.223660
H	-2.036295	0.499133	3.116532
H	-3.939664	0.397461	4.673508
H	-6.203535	1.099246	3.923999
H	-6.533277	1.877720	1.590066
H	-4.648627	1.966150	0.033358
H	-0.668806	0.424374	-0.890261
H	0.837929	0.937804	-1.723731
H	-1.708141	2.419613	0.389368
H	-1.883868	-1.747586	-1.780393
H	-2.414270	-1.558410	0.594152

B-IM5

Sum of electronic and thermal Free Energies= -3364.874538 Hartree/Particle

C	-3.589987	2.031368	0.204842
C	-2.376277	1.485911	-0.205059
C	-1.575210	2.365958	-0.930005
C	-1.917955	3.671280	-1.241946
C	-3.144237	4.163768	-0.814089
C	-3.983866	3.336621	-0.085888
B	-1.770188	-0.009936	0.174466
C	-1.370278	-0.924312	-1.153227
C	-1.740961	-0.685804	-2.475883
C	-1.326853	-1.474755	-3.545810
C	-0.504833	-2.568523	-3.316263
C	-0.133262	-2.866872	-2.013632
C	-0.582745	-2.061558	-0.974641
F	-2.539709	0.348202	-2.794785
F	-1.706327	-1.184018	-4.797217
F	-0.075468	-3.324856	-4.333218
F	0.683731	-3.910127	-1.771525
F	-0.196613	-2.441283	0.268356
F	-0.362727	1.947558	-1.389160
F	-1.087086	4.457714	-1.944997
F	-3.503912	5.421710	-1.096386
F	-5.165511	3.802751	0.342119
F	-4.470656	1.316611	0.935015
C	-2.804780	-0.920287	1.091928
C	-2.643430	-1.232019	2.435700
C	-3.507308	-2.041893	3.163461
C	-4.614646	-2.584982	2.531373
C	-4.835936	-2.298952	1.189917
C	-3.941198	-1.484455	0.511291
F	-1.587873	-0.725847	3.149244
F	-4.231474	-1.218483	-0.778642
F	-5.910068	-2.806985	0.571592
F	-5.463224	-3.368814	3.205969
F	-3.279609	-2.299260	4.459693
O	-0.468092	0.256001	0.911167
C	2.240663	0.378500	-1.167956
N	2.142592	0.533600	0.364132
Si	2.688765	-0.923590	1.441797
C	3.539821	-0.132122	-1.737216
C	3.679979	-1.490211	-2.053128
C	4.850498	-1.966394	-2.640379
C	5.895278	-1.090080	-2.924804

C	5.757709	0.267071	-2.637408
C	4.585296	0.743037	-2.057389
C	2.571177	1.856735	0.863738
C	3.920841	2.197640	0.941729
C	4.279144	3.464933	1.396856
C	3.301500	4.380773	1.777300
C	1.956518	4.027912	1.702075
C	1.584975	2.766970	1.242818
C	4.463153	-0.890398	2.004229
C	4.763615	-0.399195	3.286940
C	6.068505	-0.418548	3.771020
C	7.095151	-0.932640	2.981698
C	6.814577	-1.431620	1.710688
C	5.509823	-1.414490	1.226196
H	3.973755	-0.001065	3.915151
H	6.282514	-0.037879	4.763090
H	8.111448	-0.950832	3.358949
H	7.611030	-1.838938	1.098511
H	5.309200	-1.809544	0.237036
H	1.428377	-0.298791	-1.426733
H	4.686242	1.489061	0.660346
H	5.328084	3.729945	1.457805
H	3.586767	5.364222	2.131845
H	1.188835	4.734011	1.995131
H	0.542341	2.483918	1.178248
H	2.862860	-2.177708	-1.864385
H	4.936568	-3.017739	-2.889298
H	6.802984	-1.458181	-3.389096
H	6.555988	0.958068	-2.882670
H	4.472718	1.804507	-1.869510
H	1.081791	0.483232	0.531889
H	-0.590796	0.116837	1.854409
H	1.989227	1.359023	-1.567718
H	1.797964	-0.744086	2.604094
H	2.358893	-2.095391	0.618198

B-TS4

Sum of electronic and thermal Free Energies= -3364.866229 Hartree/Particle

C	-5.378972	-2.271669	0.111434
C	-4.066567	-2.306786	-0.389292
C	-3.774516	-3.183910	-1.447240
C	-4.768845	-3.984352	-2.000805
C	-6.068195	-3.929051	-1.499018
C	-6.372555	-3.075814	-0.440149

Si	-2.723910	-1.300462	0.410456
N	-2.204440	0.242491	-0.578994
C	-2.864408	0.464064	-1.879876
C	-4.253503	0.486267	-1.987519
C	-4.843654	0.719298	-3.227051
C	-4.054174	0.931612	-4.354357
C	-2.666859	0.920165	-4.237728
C	-2.067689	0.690763	-3.001703
C	-2.043244	1.550095	0.239866
C	-3.284595	2.141981	0.851327
C	-3.562056	1.947738	2.210681
C	-4.677283	2.537392	2.800091
C	-5.526020	3.338964	2.040132
C	-5.244429	3.563966	0.693940
C	-4.127461	2.976755	0.106247
O	0.383435	-0.426206	-0.945776
B	1.585994	-0.177786	-0.065793
C	2.926562	-0.920045	-0.723510
C	3.158860	-0.847155	-2.094472
C	4.264536	-1.378471	-2.742272
C	5.232374	-2.026432	-1.988803
C	5.063229	-2.123837	-0.615309
C	3.933353	-1.576593	-0.015335
F	2.258198	-0.204683	-2.903097
F	4.406546	-1.269209	-4.071369
F	6.312346	-2.550496	-2.579583
F	5.990621	-2.750162	0.121356
F	3.856758	-1.728040	1.320172
C	1.999332	1.435942	-0.005401
C	3.011485	1.876497	0.848639
C	3.463606	3.186546	0.912876
C	2.896452	4.143383	0.080450
C	1.890472	3.762044	-0.792193
C	1.475591	2.434083	-0.819044
F	3.596631	0.999358	1.689231
F	0.475360	2.171763	-1.711248
F	1.322080	4.671916	-1.599800
F	3.312867	5.414275	0.124128
F	4.434287	3.540002	1.765814
C	1.115341	-0.801501	1.392090
C	0.628155	-0.060330	2.463876
C	0.136665	-0.619765	3.640109
C	0.125512	-1.997406	3.786781
C	0.587001	-2.787934	2.742082

C	1.048595	-2.183685	1.580213
F	0.553045	1.293992	2.401419
F	-0.353673	0.163105	4.615960
F	-0.343941	-2.558372	4.907017
F	0.554676	-4.123058	2.857088
F	1.419196	-3.022001	0.592921
H	-2.765129	-3.248432	-1.840233
H	-4.529450	-4.655893	-2.817171
H	-6.840950	-4.557247	-1.927419
H	-7.379865	-3.041608	-0.041159
H	-5.627768	-1.617259	0.940971
H	-1.309642	1.319383	1.010150
H	-4.877005	0.326417	-1.119659
H	-5.924120	0.731145	-3.306848
H	-4.517829	1.108827	-5.317589
H	-2.042452	1.094492	-5.105699
H	-0.990994	0.717513	-2.909441
H	-2.886304	1.356637	2.818756
H	-4.872248	2.383147	3.854954
H	-6.390796	3.803715	2.499734
H	-5.884794	4.210560	0.105064
H	-3.900307	3.179748	-0.933623
H	-1.176107	0.000041	-0.781897
H	0.650472	-0.362100	-1.867592
H	-1.577062	2.244436	-0.457782
H	-3.161211	-0.779738	1.716332
H	-1.455635	-2.038630	0.473244

B-IM6

Sum of electronic and thermal Free Energies= -3364.877203 Hartree/Particle

C	3.775441	3.824137	-0.327390
C	2.656206	3.004779	-0.098647
C	1.374476	3.525938	-0.350678
C	1.225090	4.825864	-0.824792
C	2.345094	5.624486	-1.049723
C	3.621067	5.124151	-0.800029
Si	2.913524	1.306045	0.603872
N	2.439855	0.005045	-0.678929
C	3.094141	0.183742	-1.989609
C	4.468356	0.398087	-2.078477
C	5.059077	0.557265	-3.330396
C	4.284722	0.502545	-4.485895
C	2.913234	0.281304	-4.388353
C	2.313617	0.118892	-3.142507

C	2.454495	-1.460452	-0.182446
C	3.722573	-1.922401	0.484410
C	3.817937	-1.922614	1.881513
C	4.975275	-2.371022	2.512890
C	6.048188	-2.834726	1.755205
C	5.953914	-2.863839	0.364885
C	4.796383	-2.416512	-0.266047
O	-0.213966	0.544179	-0.783624
B	-1.358862	-0.056095	0.004151
C	-2.788635	0.672810	-0.445950
C	-3.054176	0.904685	-1.793084
C	-4.227852	1.454637	-2.287585
C	-5.232609	1.797238	-1.394386
C	-5.031840	1.581483	-0.038659
C	-3.833894	1.030465	0.405721
F	-2.116967	0.573474	-2.735629
F	-4.399541	1.651509	-3.602801
F	-6.377960	2.329409	-1.835353
F	-5.994796	1.911659	0.832124
F	-3.730806	0.865510	1.737654
C	-1.589901	-1.668765	-0.340764
C	-2.536876	-2.412477	0.365211
C	-2.841334	-3.739939	0.101201
C	-2.182498	-4.396666	-0.930872
C	-1.235291	-3.706122	-1.669069
C	-0.969818	-2.374495	-1.364958
F	-3.203450	-1.836207	1.385811
F	-0.017177	-1.792469	-2.151386
F	-0.580054	-4.322775	-2.665651
F	-2.455943	-5.677319	-1.204465
F	-3.756475	-4.394922	0.827451
C	-0.915126	0.235569	1.569873
C	-0.345685	-0.692729	2.435366
C	0.114446	-0.385630	3.712212
C	0.016054	0.914841	4.180523
C	-0.528900	1.887435	3.352227
C	-0.963734	1.533014	2.082389
F	-0.144709	-1.978153	2.049098
F	0.690714	-1.329835	4.474958
F	0.456244	1.232455	5.402820
F	-0.612182	3.154182	3.780402
F	-1.440996	2.543951	1.324144
H	0.494252	2.917316	-0.183522
H	0.231597	5.216538	-1.012026

H	2.223148	6.637904	-1.415403
H	4.493125	5.745077	-0.970516
H	4.774964	3.448873	-0.132893
H	1.613506	-1.538522	0.504425
H	5.080547	0.432279	-1.187457
H	6.127508	0.725070	-3.396943
H	4.747480	0.630108	-5.457291
H	2.302298	0.232298	-5.281684
H	1.252574	-0.076904	-3.072125
H	2.974038	-1.597957	2.480774
H	5.031296	-2.371106	3.595128
H	6.946858	-3.189922	2.246309
H	6.776035	-3.248572	-0.227662
H	4.720539	-2.463544	-1.346334
H	1.392552	0.190695	-0.803380
H	-0.495089	0.683747	-1.693542
H	2.220706	-2.056125	-1.063390
H	4.336678	1.083490	0.919875
H	2.040295	0.942265	1.731727

$(C_6F_5)_3OH^-$

Sum of electronic and thermal Free Energies= -2284.743465 Hartree/Particle

C	1.572983	-2.039154	-0.920264
C	0.435175	-1.476078	-0.339269
C	-0.154370	-2.259640	0.647889
C	0.305524	-3.521271	1.011201
C	1.424145	-4.047117	0.385463
C	2.066616	-3.295831	-0.586328
B	-0.077780	0.015565	-0.887553
C	1.051455	1.127584	-0.339483
C	1.671106	2.078244	-1.142483
C	2.653304	2.956036	-0.695144
C	3.053294	2.910444	0.630155
C	2.453282	1.995303	1.483436
C	1.476742	1.142327	0.987764
F	1.321282	2.231474	-2.449935
F	3.214723	3.852080	-1.530206
F	4.001771	3.748594	1.086373
F	2.821316	1.955224	2.778311
F	0.909167	0.309849	1.888586
F	-1.232460	-1.821501	1.334762
F	-0.318164	-4.236977	1.968550
F	1.887264	-5.265274	0.723905
F	3.169658	-3.789537	-1.185130

F	2.291239	-1.362381	-1.838587
O	-0.125170	-0.101475	-2.339419
C	-1.625626	0.417774	-0.376431
C	-2.679543	-0.423271	-0.742511
C	-4.016846	-0.135342	-0.511334
C	-4.360985	1.055072	0.115088
C	-3.356608	1.926704	0.496383
C	-2.026290	1.594682	0.245450
F	-2.430455	-1.603813	-1.342921
F	-4.989057	-0.993309	-0.880612
F	-5.653040	1.355625	0.345478
F	-3.677004	3.089418	1.100220
F	-1.125050	2.524849	0.647661
O	0.009406	0.746288	-2.762469

$PhH_2C\text{-}N^+H(Ph)$ (SiH_2Ph)

Sum of electronic and thermal Free Energies= -1080.035781 Hartree/Particle

C	-2.973143	-0.220496	1.217587
C	-2.446388	-1.126103	0.277937
C	-3.328983	-1.778791	-0.603941
C	-4.695533	-1.521893	-0.555393
C	-5.199218	-0.616803	0.377095
C	-4.339786	0.031334	1.263812
Si	-0.641897	-1.498494	0.202334
N	0.135505	-0.210808	-0.996555
C	0.081576	1.184888	-0.498931
C	0.660664	1.529959	0.719430
C	0.591911	2.855609	1.145133
C	-0.047780	3.816649	0.366140
C	-0.623790	3.456939	-0.850306
C	-0.558987	2.137214	-1.287806
C	1.494135	-0.606438	-1.648137
C	2.647000	-0.757877	-0.698954
C	2.906973	-1.990220	-0.085600
C	3.992826	-2.136363	0.772674
C	4.838925	-1.055686	1.015317
C	4.602687	0.167803	0.391296
C	3.513867	0.315922	-0.463048
H	-2.955055	-2.503983	-1.320253
H	-5.366686	-2.033861	-1.234531
H	-6.264587	-0.422765	0.419397
H	-4.736636	0.726258	1.994174
H	-2.318540	0.285467	1.919071
H	1.289672	-1.541868	-2.171050

H	1.168966	0.793281	1.325751
H	1.042716	3.132793	2.090159
H	-0.098613	4.843685	0.706339
H	-1.125283	4.198610	-1.459549
H	-1.012011	1.858279	-2.234267
H	2.278127	-2.848578	-0.298049
H	4.188952	-3.095709	1.236147
H	5.690637	-1.172355	1.674818
H	5.272469	1.002448	0.560112
H	3.344216	1.266217	-0.956966
H	-0.520769	-0.229906	-1.782089
H	1.688563	0.172645	-2.385793
H	0.111901	-1.338942	1.453842
H	-0.341756	-2.751024	-0.519885

B-TS5

Sum of electronic and thermal Free Energies= -3364.851046 Hartree/Particle

C	2.502978	-3.505122	-1.865658
C	1.370791	-2.674159	-1.820450
C	0.123682	-3.237016	-2.146397
C	0.010575	-4.580106	-2.492026
C	1.143847	-5.391076	-2.513950
C	2.389784	-4.851835	-2.202619
Si	1.548639	-0.839222	-1.489141
N	2.600119	-0.572786	0.658964
C	3.738287	-1.446499	0.809182
C	4.906613	-1.262698	0.063408
C	5.964714	-2.158702	0.206299
C	5.867310	-3.242560	1.075411
C	4.699631	-3.428534	1.812402
C	3.641688	-2.534432	1.683115
C	2.788366	0.848816	1.143994
C	3.746029	1.723993	0.369347
C	3.369090	2.322692	-0.837505
C	4.246170	3.157715	-1.523538
C	5.513494	3.417286	-1.004648
C	5.894476	2.842434	0.205154
C	5.014948	2.003729	0.885990
O	0.078353	-0.699071	-0.294202
B	-1.177102	0.239232	0.026340
C	-2.546199	-0.584337	-0.405041
C	-2.673932	-1.938597	-0.103157
C	-3.799232	-2.706523	-0.362300
C	-4.905204	-2.096415	-0.937053

C	-4.851627	-0.741444	-1.230986
C	-3.694885	-0.016766	-0.960182
F	-1.641611	-2.591990	0.510433
F	-3.829521	-4.010173	-0.058815
F	-6.007354	-2.803747	-1.198049
F	-5.915743	-0.141300	-1.775135
F	-3.745605	1.290829	-1.265687
C	-1.307297	0.413246	1.668176
C	-2.236474	1.323097	2.180479
C	-2.492499	1.496663	3.532697
C	-1.812088	0.719560	4.462391
C	-0.893228	-0.214312	4.012044
C	-0.676045	-0.347399	2.645109
F	-2.938035	2.099414	1.333262
F	0.233006	-1.318970	2.308197
F	-0.229014	-0.982241	4.885536
F	-2.042532	0.868807	5.768929
F	-3.386285	2.398927	3.949609
C	-0.889413	1.618003	-0.801407
C	-0.374896	2.784044	-0.236589
C	-0.144342	3.955102	-0.950773
C	-0.418603	3.987607	-2.309321
C	-0.907010	2.845285	-2.930392
C	-1.124549	1.701940	-2.175929
F	-0.036953	2.830013	1.072782
F	0.353273	5.038384	-0.343006
F	-0.197557	5.098063	-3.016943
F	-1.151954	2.856335	-4.245602
F	-1.569484	0.624938	-2.852498
H	-0.765485	-2.616837	-2.151388
H	-0.959822	-4.993037	-2.742958
H	1.055823	-6.438965	-2.778500
H	3.274506	-5.478169	-2.224077
H	3.480990	-3.098985	-1.635635
H	1.794001	1.296022	1.135096
H	4.991314	-0.432388	-0.621676
H	6.868686	-2.006168	-0.372238
H	6.693933	-3.935671	1.178698
H	4.610157	-4.267120	2.493087
H	2.735853	-2.679628	2.263126
H	2.378192	2.149866	-1.241851
H	3.935571	3.615169	-2.455726
H	6.194268	4.073244	-1.534989
H	6.873248	3.049820	0.622462

H	5.316842	1.560479	1.828848
H	1.868788	-0.935077	1.262839
H	-0.059952	-1.551374	0.146818
H	3.115410	0.799731	2.187378
H	2.968161	-0.524796	-1.785978
H	0.845037	0.037205	-2.444976

B-IM7

Sum of electronic and thermal Free Energies= -3364.895429 Hartree/Particle

C	-1.901890	3.336898	-1.966462
C	-0.725986	2.780054	-2.497963
C	0.079553	3.573206	-3.336094
C	-0.272095	4.888181	-3.621482
C	-1.439994	5.426812	-3.082476
C	-2.253989	4.651891	-2.259359
Si	-0.247816	1.025064	-2.144600
N	-4.371622	0.087900	1.627738
C	-4.820552	1.203106	0.926460
C	-5.764518	1.106260	-0.110660
C	-6.194085	2.249598	-0.780068
C	-5.702749	3.508360	-0.443695
C	-4.754076	3.607692	0.576248
C	-4.310936	2.476337	1.248110
C	-5.161627	-1.134399	1.715970
C	-4.921378	-2.143803	0.602588
C	-3.626925	-2.435349	0.163630
C	-3.409025	-3.414823	-0.801403
C	-4.486060	-4.112085	-1.348311
C	-5.779944	-3.824095	-0.922949
C	-5.993212	-2.846515	0.048082
O	0.947145	1.108812	-0.854659
B	1.662061	-0.066457	0.009098
C	3.128699	0.546183	0.420130
C	3.242290	1.860210	0.865053
C	4.419876	2.450648	1.295680
C	5.580392	1.688174	1.303532
C	5.527492	0.366485	0.882719
C	4.320613	-0.177254	0.454045
F	2.124979	2.654902	0.902778
F	4.446659	3.724773	1.700976
F	6.733156	2.221529	1.712632
F	6.640444	-0.373654	0.888976
F	4.358807	-1.462099	0.064144
C	0.818360	-0.288355	1.397484

C	1.258345	-1.271534	2.285399
C	0.671729	-1.527007	3.515570
C	-0.418004	-0.763652	3.915613
C	-0.882427	0.235899	3.076575
C	-0.267163	0.455494	1.848992
F	2.306001	-2.044359	1.940501
F	-0.791204	1.460944	1.102586
F	-1.937700	0.981591	3.458921
F	-1.009049	-0.987174	5.091698
F	1.136842	-2.493939	4.312142
C	1.668460	-1.314892	-1.036659
C	0.847639	-2.439672	-0.948323
C	0.876779	-3.481388	-1.869514
C	1.743683	-3.418868	-2.949821
C	2.568144	-2.310097	-3.095734
C	2.507294	-1.293264	-2.155025
F	-0.054154	-2.568495	0.045177
F	0.056684	-4.531907	-1.733932
F	1.776927	-4.405269	-3.845906
F	3.394451	-2.227689	-4.143898
F	3.302075	-0.227782	-2.376074
H	0.983188	3.160406	-3.773960
H	0.357468	5.489342	-4.267409
H	-1.717537	6.450079	-3.309630
H	-3.167186	5.063113	-1.846602
H	-2.551105	2.750369	-1.325232
H	-4.905869	-1.607372	2.669573
H	-6.152410	0.139024	-0.402187
H	-6.926480	2.148959	-1.573898
H	-6.055918	4.394064	-0.958515
H	-4.360637	4.577905	0.861176
H	-3.574904	2.566981	2.039553
H	-2.788584	-1.890319	0.581808
H	-2.397702	-3.644275	-1.115746
H	-4.315476	-4.874648	-2.099898
H	-6.623977	-4.358055	-1.345519
H	-7.004631	-2.627901	0.377985
H	-3.864512	0.319609	2.467251
H	0.976219	1.955773	-0.378598
H	-6.233889	-0.902137	1.763638
H	-1.358277	0.194680	-1.645602
H	0.464988	0.411044	-3.277926

C-TS1

Sum of electronic and thermal Free Energies= -2841.934007 Hartree/Particle

C	-0.526771	0.207396	2.338860
C	0.365551	-0.462915	1.511203
C	1.157971	-1.411169	2.161288
C	1.075329	-1.690291	3.516688
C	0.162027	-0.992928	4.298235
C	-0.645750	-0.036904	3.703524
B	0.646129	-0.176620	-0.072428
C	0.260400	-1.403077	-1.107827
C	0.382685	-1.179556	-2.479422
C	0.074611	-2.105189	-3.462269
C	-0.413683	-3.348901	-3.079955
C	-0.580267	-3.621005	-1.731386
C	-0.246757	-2.657918	-0.782621
F	0.838906	0.029796	-2.916323
F	0.229330	-1.815812	-4.759442
F	-0.734878	-4.260429	-4.001281
F	-1.091394	-4.798675	-1.347461
F	-0.495452	-3.004085	0.498552
F	2.056050	-2.121215	1.449514
F	1.859562	-2.618925	4.077244
F	0.062307	-1.244331	5.607213
F	-1.532415	0.644395	4.442781
F	-1.355573	1.156928	1.841860
O	-0.229359	1.036002	-0.583541
C	2.196584	0.363705	-0.212107
C	2.549175	1.594397	0.347234
C	3.831837	2.124438	0.303184
C	4.844143	1.399693	-0.310299
C	4.551893	0.161669	-0.863581
C	3.252075	-0.330008	-0.803063
F	1.623488	2.341362	0.992667
F	4.101167	3.317435	0.851596
F	6.086686	1.888102	-0.363403
F	5.522950	-0.548578	-1.450981
F	3.060248	-1.543769	-1.353220
N	-2.507828	2.069877	-0.573286
C	-3.713879	1.681554	-0.343962
C	-4.151727	0.332932	-0.018627
C	-5.507834	0.155084	0.304644
C	-5.995470	-1.100740	0.644151
C	-5.133683	-2.195525	0.663376
C	-3.784690	-2.033538	0.339169
C	-3.296380	-0.781090	-0.002344

C	-2.258750	3.428910	-0.928611
C	-3.073898	4.112813	-1.838358
C	-2.790382	5.435640	-2.163697
C	-1.694643	6.079829	-1.592908
C	-0.873858	5.390915	-0.701292
C	-1.142632	4.066147	-0.373234
H	-1.308370	1.360208	-0.483568
H	-3.902045	3.601418	-2.315331
H	-3.419153	5.957659	-2.875615
H	-1.474466	7.108901	-1.851161
H	-0.016295	5.883603	-0.258439
H	-0.508260	3.529254	0.319849
H	-4.507994	2.430702	-0.374652
H	0.072716	1.272967	-1.469986
H	-2.254449	-0.669114	-0.263823
H	-3.112964	-2.882857	0.358076
H	-5.509622	-3.176535	0.929811
H	-7.042090	-1.225865	0.894612
H	-6.176179	1.009600	0.293875

CD-IM3

Sum of electronic and thermal Free Energies= -2841.935561 Hartree/Particle

C	-0.720842	0.385162	2.199043
C	0.295240	-0.267784	1.512507
C	1.149518	-1.011527	2.329470
C	1.015705	-1.115572	3.705662
C	-0.022228	-0.443421	4.339252
C	-0.898449	0.311855	3.577587
B	0.632720	-0.153735	-0.094965
C	0.520494	-1.595286	-0.923599
C	0.758745	-1.584429	-2.298014
C	0.637441	-2.684618	-3.131222
C	0.221904	-3.894667	-2.589181
C	-0.059380	-3.960031	-1.234469
C	0.091984	-2.826441	-0.439444
F	1.138410	-0.421677	-2.897438
F	0.897775	-2.593926	-4.442605
F	0.076199	-4.972191	-3.368129
F	-0.511407	-5.106410	-0.701095
F	-0.263619	-2.988937	0.857360
F	2.169255	-1.694517	1.771488
F	1.868409	-1.854284	4.427908
F	-0.175380	-0.528412	5.665933
F	-1.909513	0.966559	4.171435

F	-1.636571	1.151344	1.546813
O	-0.362160	0.760491	-0.792468
C	2.135971	0.548949	-0.203044
C	2.291398	1.881848	0.179163
C	3.493780	2.574184	0.125522
C	4.634179	1.916410	-0.312150
C	4.543213	0.582783	-0.681911
C	3.315393	-0.068735	-0.617063
F	1.234100	2.585555	0.658732
F	3.563887	3.862237	0.498579
F	5.805865	2.559670	-0.372336
F	5.639781	-0.065376	-1.098610
F	3.327484	-1.365289	-0.983467
N	-2.768846	1.866837	-0.894694
C	-3.928540	1.323670	-0.687907
C	-4.197812	-0.040985	-0.313654
C	-5.540609	-0.375436	-0.046179
C	-5.877682	-1.660741	0.350436
C	-4.878965	-2.625061	0.485781
C	-3.544585	-2.307783	0.217684
C	-3.199738	-1.027421	-0.185098
C	-2.571403	3.221694	-1.295346
C	-3.507569	3.899661	-2.081619
C	-3.271666	5.225201	-2.427423
C	-2.106960	5.866019	-2.005265
C	-1.169445	5.173609	-1.241701
C	-1.390839	3.847278	-0.885979
H	-1.860319	1.326316	-0.735469
H	-4.390614	3.394202	-2.454129
H	-3.990330	5.751974	-3.043746
H	-1.926373	6.897532	-2.283287
H	-0.257962	5.661840	-0.918681
H	-0.670698	3.300071	-0.292364
H	-4.790238	1.976737	-0.795730
H	-0.029232	0.895730	-1.686465
H	-2.167295	-0.789967	-0.404119
H	-2.772301	-3.057283	0.334991
H	-5.138096	-3.629041	0.801354
H	-6.910735	-1.911642	0.557738
H	-6.311816	0.380999	-0.144801

PhHC=N^{+}HPh

Sum of electronic and thermal Free Energies= -557.091258 Hartree/Particle

C	0.480744	0.462418	-0.084365

N	-0.482362	-0.411507	0.044323
H	-0.220795	-1.388188	0.144372
C	-1.890291	-0.173527	0.036931
C	-2.719536	-1.244993	-0.302404
C	-2.421266	1.075642	0.365521
C	-4.095697	-1.054686	-0.338033
H	-2.294969	-2.211612	-0.552588
C	-3.798839	1.251747	0.320999
H	-1.785242	1.891552	0.686150
C	-4.636168	0.193029	-0.032531
H	-4.743227	-1.880179	-0.605511
H	-4.220587	2.214499	0.581377
H	-5.708995	0.338548	-0.057233
C	1.884245	0.187421	-0.025609
C	2.420836	-1.080363	0.293662
C	2.760409	1.256541	-0.312659
C	3.790244	-1.265916	0.310099
H	1.778445	-1.917231	0.546207
C	4.132792	1.060711	-0.295841
H	2.354942	2.233139	-0.552493
C	4.646982	-0.197982	0.013294
H	4.201840	-2.235975	0.558890
H	4.800740	1.882709	-0.519924
H	5.719354	-0.352295	0.030312
H	0.168299	1.485339	-0.264215

D-TS1

Sum of electronic and thermal Free Energies= -2843.130774 Hartree/Particle

C	-3.275662	-0.097545	-2.115663
N	-2.569756	-1.138638	-1.281816
C	-2.688739	-2.522201	-1.720405
C	-2.767907	-3.525609	-0.755659
C	-2.830149	-4.857475	-1.152640
C	-2.811500	-5.190272	-2.505622
C	-2.724405	-4.182946	-3.462063
C	-2.660471	-2.845232	-3.075598
H	-2.627035	0.148018	-2.956656
H	-2.755531	-3.270292	0.297954
H	-2.890891	-5.634179	-0.399778
H	-2.860678	-6.228359	-2.811480
H	-2.703814	-4.432766	-4.516233
H	-2.587675	-2.071470	-3.829591
H	-2.922397	-1.066917	-0.328277
H	-4.194420	-0.542019	-2.504856

C	-3.579479	1.133259	-1.298724
C	-2.738052	2.247907	-1.338832
C	-4.707715	1.157938	-0.469803
C	-3.013149	3.364512	-0.552707
H	-1.864533	2.237099	-1.980172
C	-4.979632	2.272330	0.318692
H	-5.382708	0.307138	-0.448204
C	-4.129043	3.376087	0.280391
H	-2.348508	4.219081	-0.582849
H	-5.854529	2.281382	0.958254
H	-4.334926	4.241047	0.899444
O	-0.126445	-0.711343	-1.119615
B	0.720549	-0.016808	-0.035170
C	1.961985	-1.047292	0.324978
C	2.659808	-1.664784	-0.708803
C	2.431989	-1.351596	1.600041
C	3.729703	-2.528658	-0.529145
C	3.501132	-2.210598	1.833933
C	4.153749	-2.805653	0.763520
C	-0.353320	0.205998	1.190461
C	-0.797077	1.431500	1.682794
C	-0.964294	-0.903249	1.778009
C	-1.763304	1.555323	2.678351
C	-1.937777	-0.826810	2.763611
C	-2.341766	0.420168	3.222962
C	1.384506	1.366141	-0.639911
C	1.157395	1.895969	-1.905642
C	2.309777	2.079389	0.123111
C	1.780332	3.042421	-2.388733
C	2.959267	3.223967	-0.314373
C	2.693438	3.710502	-1.588572
H	0.373343	-0.923080	-1.915314
F	4.350555	-3.089970	-1.575488
F	5.180855	-3.635498	0.973248
F	3.906278	-2.471352	3.083451
F	2.302363	-1.417149	-2.005610
F	1.858857	-0.812799	2.692840
F	-0.632148	-2.152028	1.372664
F	-2.500725	-1.941100	3.259242
F	-3.284615	0.521627	4.164457
F	-2.159478	2.765747	3.093043
F	-0.324766	2.594683	1.195782
F	3.829998	3.866090	0.473939
F	2.584709	1.671452	1.378313

F	3.304906	4.813106	-2.033331
F	1.502521	3.503063	-3.617493
F	0.272012	1.318585	-2.767802
H	-1.328331	-0.870499	-1.189836

D-IM4

Sum of electronic and thermal Free Energies= -2843.129201 Hartree/Particle

C	3.366323	-0.331004	-2.203743
N	2.765522	0.686970	-1.244533
C	3.114135	2.083242	-1.512469
C	3.846626	2.796071	-0.569871
C	4.167149	4.127535	-0.822581
C	3.757469	4.733437	-2.007623
C	3.016622	4.009987	-2.940056
C	2.688009	2.679403	-2.695538
H	2.814767	-0.238552	-3.138870
H	4.139598	2.329535	0.364373
H	4.730717	4.689390	-0.087730
H	4.006303	5.770011	-2.200504
H	2.684313	4.481868	-3.856760
H	2.099089	2.122912	-3.414854
H	3.070566	0.443420	-0.301465
H	4.400929	-0.034190	-2.379147
C	3.280712	-1.724369	-1.638711
C	2.110946	-2.481016	-1.768925
C	4.371678	-2.260729	-0.945734
C	2.034553	-3.750914	-1.204034
H	1.253998	-2.071087	-2.290950
C	4.292775	-3.531327	-0.381310
H	5.289207	-1.687310	-0.853521
C	3.121762	-4.275456	-0.507317
H	1.121438	-4.325437	-1.298822
H	5.142422	-3.938452	0.154125
H	3.054515	-5.260335	-0.060635
O	0.237768	0.361969	-1.238930
B	-0.689157	0.043723	-0.077806
C	-1.487921	1.433435	0.359197
C	-2.030916	2.243628	-0.634480
C	-1.724224	1.881607	1.656606
C	-2.738741	3.412763	-0.396491
C	-2.428007	3.045843	1.948442
C	-2.937416	3.819589	0.915590
C	0.343816	-0.531044	1.077901
C	0.454180	-1.856905	1.490206

C	1.293414	0.319287	1.643499
C	1.409004	-2.304740	2.400676
C	2.267465	-0.081196	2.547054
C	2.323237	-1.412708	2.937190
C	-1.854282	-1.033043	-0.545051
C	-2.015081	-1.552495	-1.825528
C	-2.829559	-1.439263	0.365586
C	-3.046483	-2.414427	-2.186650
C	-3.875296	-2.295452	0.055104
C	-3.986632	-2.787673	-1.239435
H	-0.261678	0.678618	-1.997887
F	-3.228397	4.144483	-1.408223
F	-3.613272	4.943750	1.179730
F	-2.615698	3.431085	3.218200
F	-1.893945	1.889799	-1.947188
F	-1.265352	1.192689	2.719998
F	1.332060	1.628011	1.281098
F	3.170104	0.797617	3.020224
F	3.259575	-1.828603	3.796160
F	1.473135	-3.600388	2.735083
F	-0.350896	-2.814857	0.991815
F	-4.772152	-2.655028	0.982917
F	-2.759548	-1.008981	1.642503
F	-4.986555	-3.614434	-1.565909
F	-3.139634	-2.881280	-3.441148
F	-1.147437	-1.243803	-2.829921
H	1.649038	0.563547	-1.232229

D-IM5

Sum of electronic and thermal Free Energies= -3399.840158 Hartree/Particle

C	-2.107830	-0.971335	2.791902
N	-1.806756	0.230478	1.896882
C	-1.864035	1.507426	2.633576
C	-3.096789	1.982401	3.074128
C	-3.150223	3.184283	3.773979
C	-1.981204	3.901404	4.026851
C	-0.756920	3.415218	3.577059
C	-0.691024	2.210686	2.877482
H	-1.339643	-0.945289	3.565424
H	-4.004368	1.432543	2.859099
H	-4.106474	3.562440	4.115390
H	-2.027460	4.838209	4.569469
H	0.156035	3.969992	3.757454
H	0.256552	1.839467	2.513877

H	-2.481945	0.279053	1.111024
H	-3.070293	-0.774574	3.261521
C	-2.123211	-2.296902	2.074249
C	-0.930740	-2.975761	1.795146
C	-3.342385	-2.892241	1.735617
C	-0.960866	-4.222031	1.177651
H	0.018631	-2.519926	2.044675
C	-3.370539	-4.142863	1.123077
H	-4.274596	-2.382071	1.952260
C	-2.180331	-4.808473	0.842147
H	-0.031004	-4.734318	0.960192
H	-4.322429	-4.592871	0.867866
H	-2.201027	-5.781673	0.365095
O	0.797583	-0.264590	1.311303
B	1.746122	-0.326842	0.134356
C	1.981917	1.230685	-0.416516
C	2.280319	2.228204	0.508540
C	1.904456	1.678731	-1.733095
C	2.434322	3.571306	0.195070
C	2.060964	3.011473	-2.098514
C	2.318784	3.967503	-1.128886
C	0.975029	-1.294319	-0.966059
C	1.393202	-2.536701	-1.433918
C	-0.274148	-0.902948	-1.438523
C	0.656193	-3.311058	-2.328183
C	-1.035954	-1.629311	-2.337518
C	-0.568094	-2.854898	-2.788495
C	3.239362	-0.889043	0.578326
C	3.613850	-1.306319	1.849408
C	4.276542	-0.911478	-0.354960
C	4.896768	-1.718678	2.192718
C	5.571791	-1.315071	-0.067325
C	5.886998	-1.722037	1.223391
H	1.293822	-0.273834	2.133694
F	2.675371	4.482594	1.153365
F	2.425029	5.261866	-1.464655
F	1.928417	3.391638	-3.379700
F	2.425293	1.914257	1.826702
F	1.650289	0.825251	-2.744235
F	-0.812199	0.271013	-1.013034
F	-2.230098	-1.169319	-2.769577
F	-1.294199	-3.585388	-3.643792
F	1.113170	-4.505317	-2.732414
F	2.553028	-3.089265	-1.022845

F	6.518478	-1.321497	-1.015163
F	4.027941	-0.549922	-1.630235
F	7.130050	-2.113878	1.525527
F	5.181282	-2.106113	3.444737
F	2.706032	-1.332237	2.874379
H	-0.827742	0.090845	1.503699
N	-4.096111	0.788328	-0.220919
C	-3.887388	1.305452	-1.375373
C	-2.930798	2.378422	-1.649502
C	-2.435293	3.215142	-0.639071
C	-2.518893	2.586871	-2.973272
C	-1.536821	4.226904	-0.949401
H	-2.774642	3.075581	0.378989
C	-1.603948	3.588188	-3.278512
H	-2.900143	1.942434	-3.758070
C	-1.112714	4.411142	-2.266929
H	-1.161697	4.874635	-0.165585
H	-1.268572	3.724637	-4.299440
H	-0.397818	5.190926	-2.502046
H	-4.463623	0.962770	-2.242549
C	-5.101429	-0.207598	-0.111167
C	-6.034338	-0.095294	0.928391
C	-5.170410	-1.307347	-0.976524
C	-7.036961	-1.048029	1.080456
H	-5.985678	0.765280	1.585867
C	-6.172131	-2.260953	-0.812325
H	-4.422239	-1.427626	-1.750280
C	-7.109802	-2.136225	0.210754
H	-7.765554	-0.938249	1.875921
H	-6.213152	-3.109512	-1.485967
H	-7.888755	-2.879889	0.331805

D-TS2

Sum of electronic and thermal Free Energies= -3399.826865 Hartree/Particle

C	-2.561694	-0.547790	2.746224
N	-2.146176	0.540004	1.786904
C	-1.998746	1.814740	2.466954
C	-3.128029	2.479778	2.952237
C	-2.991874	3.720541	3.570650
C	-1.733929	4.306580	3.702089
C	-0.609962	3.639842	3.219136
C	-0.737812	2.393661	2.608735
H	-1.806375	-0.587685	3.539037
H	-4.110630	2.032971	2.849937

H	-3.871642	4.230618	3.946064
H	-1.631671	5.273552	4.180462
H	0.375641	4.080968	3.313833
H	0.133091	1.869275	2.239236
H	-3.031750	0.730120	0.670090
H	-3.496114	-0.233839	3.211382
C	-2.737882	-1.920917	2.136748
C	-1.689003	-2.562985	1.467734
C	-3.940610	-2.607924	2.324331
C	-1.852884	-3.859682	0.986261
H	-0.742013	-2.051500	1.334093
C	-4.098874	-3.909708	1.854391
H	-4.759795	-2.125030	2.846458
C	-3.055143	-4.537900	1.180233
H	-1.031385	-4.345926	0.472644
H	-5.036356	-4.429945	2.015013
H	-3.174077	-5.551366	0.813780
O	0.699163	-0.321513	1.240954
B	1.734028	-0.443444	0.165324
C	2.069905	1.091723	-0.414470
C	2.353350	2.099476	0.505080
C	2.087995	1.510308	-1.742325
C	2.574995	3.428327	0.169545
C	2.314449	2.827280	-2.128075
C	2.551236	3.796822	-1.166934
C	1.018010	-1.416157	-0.978948
C	1.417990	-2.685259	-1.388099
C	-0.187001	-0.999054	-1.534930
C	0.700598	-3.465517	-2.295548
C	-0.928674	-1.732539	-2.443740
C	-0.484883	-2.988000	-2.830634
C	3.181131	-1.035622	0.715563
C	3.465447	-1.407418	2.023953
C	4.270445	-1.127512	-0.151241
C	4.713154	-1.841732	2.459182
C	5.533152	-1.555927	0.229424
C	5.758101	-1.916474	1.552265
H	1.104980	-0.416912	2.105595
F	2.786286	4.357023	1.119632
F	2.714870	5.081131	-1.524911
F	2.261764	3.183486	-3.424316
F	2.408489	1.815578	1.832331
F	1.858115	0.644033	-2.750182
F	-0.703946	0.209308	-1.190764

F	-2.094125	-1.248696	-2.939781
F	-1.195579	-3.724451	-3.695040
F	1.138937	-4.684623	-2.642583
F	2.539859	-3.257447	-0.908847
F	6.534525	-1.629810	-0.658969
F	4.110436	-0.809255	-1.453281
F	6.968849	-2.331375	1.944830
F	4.912752	-2.182499	3.741303
F	2.501382	-1.359950	2.990525
H	-1.223987	0.276981	1.402941
N	-3.788386	0.761037	-0.279087
C	-3.551947	1.329558	-1.416979
C	-2.579240	2.358096	-1.719874
C	-2.022217	3.205564	-0.748781
C	-2.220691	2.523560	-3.069905
C	-1.113251	4.183249	-1.124222
H	-2.316164	3.115670	0.287568
C	-1.290857	3.486027	-3.435180
H	-2.650632	1.870120	-3.820716
C	-0.737692	4.318119	-2.462218
H	-0.687961	4.837689	-0.373301
H	-0.991132	3.587224	-4.470728
H	-0.008676	5.068388	-2.744339
H	-4.178463	1.016437	-2.252212
C	-4.889763	-0.162609	-0.190032
C	-5.906394	0.103198	0.727459
C	-4.944203	-1.292547	-1.005437
C	-6.996557	-0.758172	0.812060
H	-5.856885	0.994538	1.341799
C	-6.037792	-2.149130	-0.909788
H	-4.130783	-1.506153	-1.687914
C	-7.064688	-1.883834	-0.007032
H	-7.795715	-0.544171	1.512182
H	-6.078501	-3.031038	-1.537763
H	-7.914042	-2.553289	0.061177

CD-TS3

Sum of electronic and thermal Free Energies= -3364.795223 Hartree/Particle

C	3.179908	0.380423	-1.701645
N	2.321678	-0.718110	-1.364461
C	2.350248	-1.902456	-2.152679
C	1.299256	-2.818392	-1.997667
C	1.307634	-4.010965	-2.707647
C	2.358383	-4.322722	-3.573006

C	3.408238	-3.424580	-3.713314
C	3.415005	-2.220661	-3.004802
H	4.224495	0.248817	-1.130505
H	0.485858	-2.578929	-1.325081
H	0.482369	-4.702068	-2.579626
H	2.356677	-5.254687	-4.125386
H	4.235230	-3.651228	-4.376838
H	4.255374	-1.549301	-3.138365
H	1.369227	-0.476145	-1.040148
H	3.560585	0.323806	-2.725516
C	2.728317	1.773664	-1.382086
C	1.839123	2.064979	-0.341308
C	3.267215	2.822872	-2.139781
C	1.497194	3.386660	-0.067817
H	1.388694	1.271098	0.237790
C	2.921646	4.140832	-1.864569
H	3.951094	2.605359	-2.954098
C	2.037751	4.424342	-0.824457
H	0.796153	3.599425	0.729567
H	3.333840	4.943249	-2.464921
H	1.760273	5.449907	-0.610827
Si	4.206468	-0.842961	0.321950
H	3.274692	-0.091805	1.162895
C	5.975999	-0.455556	0.668660
C	6.336473	0.707703	1.377858
C	6.990784	-1.337903	0.248147
C	7.669873	0.972201	1.665581
H	5.571242	1.400421	1.712844
C	8.323310	-1.070006	0.538490
H	6.734898	-2.240587	-0.297730
C	8.661003	0.084386	1.245289
H	7.938680	1.864262	2.218838
H	9.097489	-1.757772	0.219349
H	9.700567	0.291900	1.471983
H	4.040469	-2.240906	-0.095363
O	-0.462073	-0.389163	-0.838136
B	-1.624925	-0.030131	0.039914
C	-2.859287	-1.125393	-0.215736
C	-2.568923	-2.490004	-0.191894
C	-4.204516	-0.832281	-0.434887
C	-3.506333	-3.491420	-0.409808
C	-5.179381	-1.801276	-0.651408
C	-4.828337	-3.142786	-0.643492
C	-2.037181	1.527231	-0.391367

C	-1.914901	2.679196	0.375700
C	-2.419032	1.768211	-1.710425
C	-2.182718	3.959288	-0.101751
C	-2.708727	3.018214	-2.233549
C	-2.590421	4.133284	-1.413771
C	-1.221313	-0.189919	1.634620
C	-0.002645	-0.626691	2.133126
C	-2.185021	0.035856	2.620004
C	0.269801	-0.813508	3.484154
C	-1.967439	-0.141486	3.978843
C	-0.722118	-0.573484	4.419443
H	-0.787357	-0.379147	-1.744139
F	-3.148748	-4.786761	-0.387417
F	-5.752496	-4.089056	-0.854034
F	-6.456464	-1.451995	-0.867408
F	-1.309584	-2.920114	0.070597
F	-4.644474	0.442031	-0.447455
F	-2.514554	0.722933	-2.576295
F	-3.081666	3.166702	-3.513507
F	-2.842597	5.358738	-1.892631
F	-2.005288	5.031996	0.689435
F	-1.458540	2.631052	1.652299
F	-2.937584	0.102379	4.870520
F	-3.408465	0.472160	2.262436
F	-0.483853	-0.746137	5.725890
F	1.492380	-1.218441	3.882666
F	1.049173	-0.883332	1.304730

CD-IM4

Sum of electronic and thermal Free Energies= -3364.873173 Hartree/Particle

C	-2.849216	-0.755352	-1.494574
N	-2.607804	0.428045	-0.559468
C	-2.730379	1.744493	-1.241093
C	-1.850356	2.754719	-0.854104
C	-1.947617	4.010385	-1.447012
C	-2.916246	4.258953	-2.416810
C	-3.794052	3.245320	-2.790160
C	-3.710435	1.984035	-2.201862
H	-3.857393	-0.662458	-1.891286
H	-1.083702	2.555984	-0.117750
H	-1.253781	4.787323	-1.148912
H	-2.984700	5.235632	-2.880994
H	-4.551746	3.428824	-3.542656
H	-4.411280	1.216669	-2.498881

H	-1.586251	0.363766	-0.293863
H	-2.142584	-0.623839	-2.316516
C	-2.688922	-2.107785	-0.841387
C	-1.465682	-2.510208	-0.295028
C	-3.763244	-3.003394	-0.836538
C	-1.327360	-3.776012	0.266137
H	-0.622066	-1.833261	-0.317045
C	-3.622561	-4.274226	-0.282300
H	-4.710993	-2.711576	-1.277132
C	-2.405785	-4.659633	0.275015
H	-0.371966	-4.070034	0.684594
H	-4.460489	-4.961901	-0.290482
H	-2.294383	-5.647319	0.707232
Si	-3.657973	0.426581	1.029585
H	-3.348828	-0.829486	1.724841
C	-5.465242	0.525995	0.583743
C	-6.263293	-0.631327	0.607939
C	-6.086333	1.757839	0.309969
C	-7.629630	-0.563312	0.346696
H	-5.817049	-1.591360	0.843856
C	-7.451654	1.825739	0.048970
H	-5.502986	2.672117	0.305903
C	-8.223321	0.664798	0.063534
H	-8.230838	-1.464948	0.373111
H	-7.915009	2.783715	-0.157426
H	-9.287757	0.719334	-0.134948
H	-3.186403	1.646789	1.702041
O	0.155789	0.428024	-0.562835
B	1.522762	0.059279	-0.021973
C	2.533532	1.368808	-0.221916
C	2.112752	2.624809	0.215674
C	3.813031	1.357581	-0.776286
C	2.856058	3.789673	0.080888
C	4.598294	2.497120	-0.923602
C	4.115429	3.725339	-0.497098
C	1.991577	-1.269285	-0.911036
C	2.216793	-2.563824	-0.454759
C	2.055786	-1.142080	-2.298132
C	2.517654	-3.636416	-1.290781
C	2.359733	-2.171899	-3.173361
C	2.598001	-3.440696	-2.659819
C	1.449497	-0.212677	1.600253
C	0.322982	-0.102043	2.400901
C	2.620479	-0.496991	2.305951

C	0.322448	-0.266736	3.781876
C	2.676729	-0.669720	3.681019
C	1.512097	-0.552972	4.430668
H	0.299349	0.729349	-1.466181
F	2.371813	4.968351	0.507221
F	4.854032	4.832505	-0.637584
F	5.817361	2.420652	-1.475463
F	0.911093	2.770738	0.832835
F	4.371623	0.210776	-1.209081
F	1.804221	0.070586	-2.867660
F	2.413959	-1.964792	-4.497158
F	2.881226	-4.460441	-3.478449
F	2.702224	-4.863877	-0.781479
F	2.104348	-2.876901	0.857530
F	3.834487	-0.949281	4.293755
F	3.780922	-0.632428	1.634583
F	1.540021	-0.716775	5.758410
F	-0.817736	-0.148461	4.483802
F	-0.898734	0.183074	1.862922

CD-IM5

Sum of electronic and thermal Free Energies= -3364.875824 Hartree/Particle

C	-2.800221	1.498867	1.899761
N	-2.433280	0.367176	0.932891
C	-2.690377	-0.950308	1.553262
C	-1.619867	-1.813505	1.764304
C	-1.847128	-3.064320	2.332961
C	-3.134847	-3.441886	2.703811
C	-4.198870	-2.564922	2.503536
C	-3.983610	-1.316473	1.924069
H	-3.861438	1.395753	2.119268
H	-0.618221	-1.518023	1.490953
H	-1.009589	-3.735859	2.476963
H	-3.309108	-4.414111	3.149220
H	-5.203045	-2.850139	2.794201
H	-4.819098	-0.648045	1.761593
H	-1.384886	0.429978	0.743346
H	-2.237852	1.282046	2.809004
C	-2.502577	2.889838	1.398350
C	-3.542524	3.717886	0.963066
C	-1.196917	3.394480	1.412201
C	-3.280495	5.010703	0.515032
H	-4.564387	3.354754	0.988167
C	-0.931924	4.680591	0.950033

H	-0.388951	2.786851	1.800002
C	-1.972522	5.489211	0.496258
H	-4.096609	5.644109	0.186624
H	0.087394	5.047542	0.949575
H	-1.765665	6.492328	0.141837
Si	-3.023195	0.450139	-0.872379
H	-2.475263	1.715906	-1.381738
C	-4.880013	0.397632	-1.049177
C	-5.614224	1.578368	-1.255971
C	-5.567027	-0.828924	-1.097682
C	-6.989131	1.537843	-1.474303
H	-5.106518	2.536541	-1.263848
C	-6.940936	-0.870062	-1.315807
H	-5.025502	-1.760323	-0.972347
C	-7.653841	0.313809	-1.498968
H	-7.538555	2.458313	-1.635520
H	-7.453332	-1.824549	-1.353532
H	-8.723225	0.280914	-1.674040
H	-2.398679	-0.766711	-1.412601
O	0.039671	0.655312	-0.079165
B	1.342907	-0.093945	-0.210700
C	0.907871	-1.508468	-0.945421
C	0.365786	-1.460985	-2.231506
C	0.935086	-2.782062	-0.386832
C	-0.093246	-2.573020	-2.922688
C	0.484816	-3.926129	-1.039222
C	-0.028722	-3.823432	-2.321476
C	2.086773	-0.296781	1.267136
C	3.344528	-0.898172	1.342133
C	1.603166	0.150087	2.491592
C	4.071234	-1.044362	2.514357
C	2.291317	0.029957	3.695290
C	3.539147	-0.571060	3.707588
C	2.403290	0.820403	-1.118402
C	2.550111	2.178727	-0.852876
C	3.235738	0.351518	-2.134175
C	3.413797	3.032011	-1.522982
C	4.122853	1.162976	-2.835287
C	4.213902	2.513571	-2.530673
H	0.220414	1.595785	0.010409
F	-0.608485	-2.453493	-4.155929
F	-0.475469	-4.908760	-2.964700
F	0.518442	-5.119271	-0.425023
F	0.257985	-0.280284	-2.877582

F	1.362489	-2.980478	0.884600
F	0.375886	0.744229	2.600987
F	1.755508	0.486888	4.838424
F	4.219869	-0.699716	4.852308
F	5.272457	-1.637041	2.512604
F	3.906636	-1.397149	0.222822
F	4.892518	0.652451	-3.805767
F	3.223473	-0.943956	-2.498226
F	5.059871	3.305715	-3.199068
F	3.482170	4.334838	-1.208059
F	1.800598	2.759401	0.137565

CD-TS4

Sum of electronic and thermal Free Energies= -3441.274207 Hartree/Particle

C	2.920453	0.208464	-2.031132
N	1.877554	-0.646820	-2.091600
C	1.985771	-1.996760	-2.492709
C	0.829950	-2.785743	-2.421151
C	0.871160	-4.116240	-2.814764
C	2.057077	-4.681321	-3.283667
C	3.206823	-3.899061	-3.346080
C	3.181999	-2.563369	-2.951213
H	3.733079	-0.107749	-0.907140
H	-0.083405	-2.350355	-2.038503
H	-0.031725	-4.711946	-2.747015
H	2.085794	-5.719880	-3.591076
H	4.137260	-4.327340	-3.701235
H	4.098062	-1.988568	-3.000816
H	0.989197	-0.406309	-1.625112
H	3.726816	-0.027826	-2.719710
C	2.716449	1.669432	-1.856402
C	3.738027	2.524479	-2.293362
C	1.570675	2.213829	-1.264649
C	3.615156	3.901880	-2.150517
H	4.629159	2.108226	-2.752180
C	1.453162	3.593887	-1.124893
H	0.761644	1.573371	-0.933790
C	2.470548	4.439188	-1.563401
H	4.405730	4.554115	-2.502971
H	0.560078	4.007944	-0.673193
H	2.369168	5.512647	-1.453026
Si	4.104696	-0.489126	0.673976
H	3.216107	0.582774	1.161612
O	4.213192	-1.135520	2.823932

H	4.438337	-0.479767	3.494227
C	5.934552	-0.133183	0.659207
C	6.403571	1.186367	0.544532
C	6.874181	-1.174585	0.730791
C	7.769487	1.455874	0.508609
H	5.700426	2.011152	0.483039
C	8.239399	-0.904507	0.691771
H	6.539538	-2.201978	0.828573
C	8.688226	0.410521	0.580660
H	8.116310	2.479653	0.424886
H	8.952777	-1.718746	0.750696
H	9.751541	0.619982	0.551814
H	3.651801	-1.882115	0.541502
H	3.374624	-1.545295	3.090989
O	-0.785608	-0.139766	-1.107135
B	-1.804453	0.062873	-0.019777
C	-3.189195	-0.771422	-0.435283
C	-3.086339	-2.120473	-0.776197
C	-4.489857	-0.271224	-0.477119
C	-4.157924	-2.911658	-1.169155
C	-5.593994	-1.025438	-0.861946
C	-5.428129	-2.356250	-1.215019
C	-2.051442	1.710369	0.083946
C	-1.850555	2.535891	1.185878
C	-2.423572	2.392239	-1.074603
C	-2.032072	3.917708	1.156946
C	-2.621044	3.761167	-1.156155
C	-2.422211	4.536161	-0.020078
C	-1.267440	-0.597038	1.398451
C	-0.007425	-1.133704	1.626394
C	-2.136949	-0.699650	2.486721
C	0.360818	-1.732842	2.825540
C	-1.808543	-1.288602	3.700456
C	-0.536728	-1.817206	3.874514
H	-1.203988	0.132997	-1.930386
F	-3.978199	-4.202696	-1.493617
F	-6.478952	-3.096295	-1.589099
F	-6.818833	-0.480109	-0.890325
F	-1.886949	-2.750458	-0.719989
F	-4.756038	1.003619	-0.127142
F	-2.630683	1.692003	-2.223031
F	-2.989902	4.343630	-2.305992
F	-2.593212	5.863604	-0.066998
F	-1.819695	4.657257	2.256532

F	-1.449138	2.037310	2.376494
F	-2.693545	-1.345177	4.703277
F	-3.374640	-0.180122	2.399535
F	-0.180821	-2.389558	5.031159
F	1.612705	-2.254189	2.985528
F	0.967932	-1.089336	0.682481

CD-IM6

Sum of electronic and thermal Free Energies= -3441.314744 Hartree/Particle

C	2.770313	0.887550	-1.786301
N	2.536507	-0.358340	-0.944052
C	2.669556	-1.605842	-1.728531
C	1.711353	-2.602377	-1.546432
C	1.827730	-3.800556	-2.246290
C	2.891806	-4.006595	-3.120864
C	3.848243	-3.008842	-3.288722
C	3.746217	-1.806687	-2.590800
H	3.777715	0.825866	-2.190893
H	0.880323	-2.437754	-0.873211
H	1.076774	-4.568426	-2.102816
H	2.975951	-4.938208	-3.667878
H	4.682675	-3.160629	-3.963284
H	4.509499	-1.052029	-2.721986
H	1.530235	-0.322229	-0.657180
H	2.067504	0.820384	-2.620602
C	2.608311	2.195402	-1.045447
C	3.661995	3.114405	-1.036048
C	1.404501	2.537065	-0.419918
C	3.522513	4.347577	-0.401435
H	4.594505	2.869495	-1.533759
C	1.269352	3.762720	0.225963
H	0.573444	1.842802	-0.441170
C	2.327820	4.670303	0.236840
H	4.344963	5.053898	-0.409028
H	0.332932	4.008573	0.712540
H	2.216943	5.627369	0.733457
Si	3.531188	-0.491563	0.737213
H	3.044245	0.734653	1.371231
O	3.982483	-0.883671	3.230965
H	4.355093	-0.174898	3.766379
C	5.350723	-0.440695	0.328645
C	6.072554	0.762447	0.398431
C	6.048988	-1.618365	0.012970
C	7.442253	0.790964	0.144989

H	5.564017	1.684604	0.658912
C	7.417693	-1.590926	-0.240709
H	5.523038	-2.565940	-0.028316
C	8.114939	-0.385644	-0.178046
H	7.984413	1.727969	0.205736
H	7.941191	-2.509666	-0.479871
H	9.181518	-0.365203	-0.371852
H	3.043167	-1.827236	1.081806
H	3.109839	-1.055652	3.610469
O	-0.338718	-0.349804	-0.751841
B	-1.646766	-0.061899	-0.052369
C	-2.714919	-1.306428	-0.352770
C	-2.292357	-2.624530	-0.177541
C	-4.048557	-1.181868	-0.741065
C	-3.089609	-3.738026	-0.406796
C	-4.887166	-2.267682	-0.974663
C	-4.404135	-3.557413	-0.811431
C	-2.153324	1.395803	-0.681172
C	-2.256750	2.618198	-0.026596
C	-2.378075	1.473231	-2.055352
C	-2.595018	3.809936	-0.662409
C	-2.726980	2.628829	-2.735494
C	-2.840576	3.817634	-2.025638
C	-1.441917	-0.053922	1.585928
C	-0.282889	-0.406567	2.259842
C	-2.520764	0.226227	2.427511
C	-0.164844	-0.441873	3.644080
C	-2.455633	0.199095	3.813856
C	-1.258135	-0.136546	4.435306
H	-0.556018	-0.477587	-1.681316
F	-2.605297	-4.979063	-0.233215
F	-5.195146	-4.613335	-1.036659
F	-6.158177	-2.080216	-1.357202
F	-1.034494	-2.890054	0.259440
F	-4.610519	0.030211	-0.915586
F	-2.245319	0.350470	-2.814805
F	-2.939963	2.617371	-4.059195
F	-3.160855	4.954707	-2.654054
F	-2.649468	4.957891	0.031573
F	-1.973607	2.736194	1.293014
F	-3.527698	0.493317	4.560012
F	-3.709281	0.557463	1.890587
F	-1.165326	-0.165790	5.769524
F	1.014215	-0.779838	4.225151

F	0.846078	-0.756951	1.587583

CD-TS5

Sum of electronic and thermal Free Energies= -3922.735797 Hartree/Particle

C	-1.345212	-0.543258	-2.918694
N	-0.451399	0.451492	-2.808285
C	-0.654849	1.761311	-3.299928
C	0.260602	2.748926	-2.911295
C	0.113411	4.050936	-3.371663
C	-0.940879	4.390083	-4.218569
C	-1.854500	3.409622	-4.596782
C	-1.721600	2.100329	-4.142473
H	-2.480637	-0.255780	-1.987299
H	1.063855	2.486452	-2.235477
H	0.826668	4.803592	-3.056302
H	-1.052223	5.406951	-4.575834
H	-2.681642	3.660379	-5.251121
H	-2.451991	1.364695	-4.454026
H	0.356252	0.349351	-2.168353
H	-2.017771	-0.463948	-3.766149
C	-1.021874	-1.937901	-2.543869
C	-1.654245	-2.966672	-3.256186
C	-0.160330	-2.263094	-1.488334
C	-1.416383	-4.298096	-2.933209
H	-2.328888	-2.721806	-4.069851
C	0.063560	-3.596048	-1.159639
H	0.335401	-1.483347	-0.926432
C	-0.559162	-4.613969	-1.880808
H	-1.898265	-5.085613	-3.500874
H	0.720672	-3.837662	-0.333933
H	-0.374978	-5.650238	-1.621821
Si	-3.441643	-0.000487	-0.675271
H	-2.668394	-0.934820	0.163024
C	-5.045364	-0.625961	-1.407088
C	-5.305158	-2.005307	-1.484297
C	-5.988503	0.259621	-1.954182
C	-6.472639	-2.481854	-2.076636
H	-4.587657	-2.715323	-1.085619
C	-7.155074	-0.217184	-2.548562
H	-5.816980	1.329688	-1.911904
C	-7.399861	-1.587667	-2.608985
H	-6.657049	-3.549305	-2.125580
H	-7.872850	0.481673	-2.963409
H	-8.307844	-1.957808	-3.071645

H	-3.219939	1.455500	-0.637246
O	1.988501	0.453080	-1.378059
B	2.769355	0.189855	-0.125223
C	3.925849	1.378602	0.068929
C	3.550657	2.716897	-0.057040
C	5.270917	1.190122	0.384225
C	4.425526	3.787876	0.071827
C	6.182164	2.231936	0.527924
C	5.758500	3.542428	0.366850
C	3.429021	-1.327610	-0.326255
C	3.128865	-2.486301	0.379255
C	4.292456	-1.532280	-1.401807
C	3.664763	-3.735543	0.079063
C	4.862357	-2.749973	-1.737556
C	4.543899	-3.871505	-0.982396
C	1.788194	0.327271	1.201008
C	0.459002	0.733236	1.202679
C	2.328595	0.138388	2.475285
C	-0.276388	0.936653	2.364854
C	1.623678	0.307422	3.658890
C	0.298048	0.715631	3.602567
H	2.614539	0.435737	-2.109334
F	3.993613	5.051682	-0.074734
F	6.621835	4.557372	0.499173
F	7.466698	1.982290	0.822300
F	2.259262	3.046841	-0.304676
F	5.773951	-0.046346	0.573558
F	4.614205	-0.481463	-2.203845
F	5.696128	-2.862107	-2.781413
F	5.060403	-5.067614	-1.290723
F	3.296891	-4.819819	0.784315
F	2.228348	-2.479998	1.393212
F	2.198984	0.081271	4.847476
F	3.611183	-0.250025	2.598518
F	-0.420401	0.874305	4.725502
F	-1.569737	1.345897	2.297524
F	-0.226665	0.944354	0.050297
N	-4.473871	0.528471	1.474426
C	-5.230349	1.743610	1.396859
C	-6.612793	1.730114	1.191176
C	-7.310557	2.931400	1.078568
C	-6.643943	4.150442	1.161468
C	-5.264601	4.162130	1.362603
C	-4.559383	2.969470	1.480908

C	-5.132770	-0.619018	2.168743
C	-4.126083	-1.585659	2.751843
C	-3.247482	-1.170742	3.759977
C	-2.319433	-2.054745	4.302038
C	-2.268448	-3.374427	3.855334
C	-3.149376	-3.802473	2.865970
C	-4.069755	-2.911499	2.316506
H	-5.772134	-0.223697	2.966444
H	-7.146613	0.792126	1.111180
H	-8.383498	2.907997	0.924849
H	-7.192001	5.081099	1.075310
H	-4.731910	5.103280	1.435142
H	-3.487897	2.984334	1.646916
H	-3.282297	-0.150659	4.128850
H	-1.638743	-1.710112	5.071493
H	-1.545499	-4.063020	4.276858
H	-3.117380	-4.828101	2.516398
H	-4.751644	-3.249613	1.543460
H	-3.588317	0.721976	1.935128
H	-5.777963	-1.134585	1.455614

CD-IM7

Sum of electronic and thermal Free Energies= -3922.775807 Hartree/Particle

C	1.133060	0.889013	-3.007904
N	1.273777	-0.284427	-2.053328
C	1.275683	-1.583434	-2.760166
C	0.501454	-2.618852	-2.237608
C	0.507674	-3.862982	-2.862801
C	1.281978	-4.077461	-4.000286
C	2.059144	-3.040416	-4.509080
C	2.064501	-1.791313	-3.890740
H	1.981207	0.862172	-3.687942
H	-0.107135	-2.448791	-1.359414
H	-0.101411	-4.660086	-2.453083
H	1.280492	-5.045607	-4.487102
H	2.669076	-3.197530	-5.390984
H	2.688428	-1.004779	-4.292499
H	0.401381	-0.290652	-1.477661
H	0.229750	0.694248	-3.592439
C	1.064180	2.251145	-2.354106
C	1.922162	3.262864	-2.796770
C	0.112254	2.551439	-1.374189
C	1.839342	4.548349	-2.264592
H	2.652397	3.048834	-3.570399

C	0.039720	3.830855	-0.830709
H	-0.578041	1.785279	-1.043640
C	0.901764	4.832234	-1.275139
H	2.504215	5.324966	-2.625662
H	-0.698430	4.044158	-0.066857
H	0.835355	5.830178	-0.857342
Si	2.749095	-0.214889	-0.738789
H	2.343933	1.003895	-0.035181
C	4.320371	-0.048418	-1.736085
C	4.849533	1.213800	-2.055874
C	5.030805	-1.189214	-2.147042
C	6.038004	1.332226	-2.773841
H	4.329680	2.112383	-1.742153
C	6.219389	-1.071565	-2.864132
H	4.659082	-2.177288	-1.900716
C	6.722811	0.188641	-3.180897
H	6.430497	2.314531	-3.012388
H	6.753892	-1.963485	-3.171030
H	7.648391	0.279598	-3.738299
H	2.501493	-1.563375	-0.226920
O	-1.417440	-0.455333	-1.024955
B	-2.495980	-0.195487	-0.002851
C	-3.518475	-1.512201	0.066081
C	-2.975147	-2.792949	0.172456
C	-4.912844	-1.482872	0.065563
C	-3.727094	-3.959068	0.226619
C	-5.707365	-2.623903	0.125968
C	-5.111365	-3.873797	0.202046
C	-3.257542	1.190971	-0.527571
C	-3.254908	2.445199	0.072513
C	-3.864110	1.169767	-1.783023
C	-3.838892	3.574952	-0.494329
C	-4.467951	2.260404	-2.387768
C	-4.457805	3.483999	-1.730142
C	-1.845191	-0.078667	1.509785
C	-0.527191	-0.343836	1.851825
C	-2.667939	0.201461	2.603252
C	-0.039971	-0.304969	3.152866
C	-2.227479	0.256105	3.918286
C	-0.890330	0.002655	4.199760
H	-1.871577	-0.655363	-1.850260
F	-3.130072	-5.159897	0.311214
F	-5.859999	-4.982227	0.255807
F	-7.044526	-2.527918	0.110421

F	-1.630605	-2.965032	0.248994
F	-5.582975	-0.315527	0.004533
F	-3.874591	0.009997	-2.496777
F	-5.043419	2.154400	-3.594372
F	-5.018290	4.561248	-2.292809
F	-3.773032	4.760606	0.132813
F	-2.618862	2.661208	1.248990
F	-3.070548	0.549209	4.916837
F	-3.975489	0.448291	2.400334
F	-0.433562	0.053202	5.457279
F	1.264369	-0.574760	3.403449
F	0.398512	-0.675642	0.911961
N	4.108936	-0.409007	1.534717
C	4.616873	-1.734067	1.637310
C	5.933972	-2.043657	1.279254
C	6.384171	-3.360991	1.346156
C	5.535387	-4.383405	1.760326
C	4.222279	-4.075846	2.114243
C	3.763871	-2.764749	2.056117
C	5.043162	0.702887	1.851051
C	4.310901	1.947389	2.301923
C	3.560182	1.937932	3.483988
C	2.893560	3.082207	3.911341
C	2.978287	4.259246	3.169057
C	3.731702	4.283416	1.998890
C	4.390832	3.133074	1.568593
H	5.735548	0.378897	2.638486
H	6.606864	-1.265490	0.942485
H	7.408989	-3.584183	1.070830
H	5.891944	-5.405207	1.812368
H	3.549586	-4.858588	2.445879
H	2.745680	-2.529362	2.346053
H	3.494208	1.032460	4.078506
H	2.312253	3.055466	4.825820
H	2.460336	5.150914	3.502921
H	3.803158	5.194847	1.416570
H	4.976078	3.157485	0.655567
H	3.267923	-0.320429	2.097702
H	5.641196	0.926474	0.965085

CD-TS6

Sum of electronic and thermal Free Energies= -3364.849382 Hartree/Particle

C	3.347653	-1.564016	1.628719
N	2.648368	-0.310720	1.189630

C	3.299833	0.927963	1.576161
C	2.500944	2.059102	1.771683
C	3.082215	3.273210	2.117900
C	4.463541	3.372757	2.278520
C	5.255489	2.243842	2.095698
C	4.681785	1.021323	1.745705
H	4.171808	-1.749338	0.940813
H	1.425725	1.990238	1.665400
H	2.448089	4.140135	2.262182
H	4.915253	4.319430	2.549746
H	6.329749	2.305646	2.226510
H	5.317468	0.158337	1.602005
H	1.726660	-0.295648	1.619325
H	3.768001	-1.387375	2.623296
C	2.418828	-2.757223	1.671093
C	2.469754	-3.745905	0.682503
C	1.514711	-2.911126	2.730327
C	1.619326	-4.849139	0.735872
H	3.187895	-3.657912	-0.123624
C	0.663869	-4.010895	2.782251
H	1.470833	-2.166960	3.517593
C	0.710710	-4.980117	1.781703
H	1.668827	-5.605094	-0.039263
H	-0.033492	-4.111770	3.605658
H	0.042818	-5.832588	1.818722
Si	1.949357	-0.267662	-1.029433
H	1.196459	-0.989136	-2.088982
C	3.672620	-0.883462	-1.548748
C	3.783869	-2.091438	-2.256447
C	4.823980	-0.084242	-1.439870
C	4.999043	-2.509846	-2.795063
H	2.901781	-2.705573	-2.409677
C	6.038428	-0.490564	-1.990131
H	4.770734	0.878386	-0.946241
C	6.131620	-1.710280	-2.657642
H	5.057840	-3.448102	-3.335708
H	6.909032	0.151010	-1.907877
H	7.076518	-2.026206	-3.085397
H	1.958925	1.197591	-1.114880
O	0.317567	-0.380272	0.022710
B	-1.117680	0.274096	-0.221508
C	-0.812467	1.727848	-0.909882
C	-0.574608	1.885372	-2.277275
C	-0.693564	2.906355	-0.172722

C	-0.291304	3.102670	-2.880720
C	-0.403679	4.145536	-0.731908
C	-0.211891	4.248225	-2.100794
C	-1.879336	0.397824	1.244030
C	-3.202766	0.843550	1.280619
C	-1.361833	0.081244	2.494899
C	-3.958203	0.951284	2.440478
C	-2.076635	0.164800	3.683950
C	-3.391226	0.602022	3.658748
C	-2.006809	-0.800540	-1.115306
C	-1.934921	-2.163484	-0.836596
C	-2.939447	-0.476902	-2.103092
C	-2.667196	-3.148754	-1.480983
C	-3.701602	-1.426084	-2.777132
C	-3.563749	-2.772121	-2.470128
H	0.166339	-1.284719	0.340672
F	-0.073786	3.179313	-4.198948
F	0.068718	5.428374	-2.658438
F	-0.290175	5.232826	0.043662
F	-0.560313	0.812378	-3.092396
F	-0.812059	2.900418	1.175798
F	-0.067837	-0.328446	2.645027
F	-1.501685	-0.170346	4.848173
F	-4.098750	0.691807	4.788335
F	-5.221610	1.388608	2.395818
F	-3.809372	1.220833	0.138880
F	-4.571985	-1.050846	-3.721382
F	-3.161076	0.798982	-2.458045
F	-4.288108	-3.692772	-3.112410
F	-2.523264	-4.440534	-1.154687
F	-1.099907	-2.610491	0.155248

CD-IM8

Sum of electronic and thermal Free Energies= -3364.895669 Hartree/Particle

C	5.611076	-0.668326	-0.302027
N	4.218619	-0.918037	-0.644704
C	3.672335	-2.192682	-0.654232
C	2.385430	-2.393503	-1.194833
C	1.787736	-3.645746	-1.175999
C	2.448454	-4.742843	-0.616846
C	3.723175	-4.557054	-0.089410
C	4.336736	-3.305242	-0.106303
H	5.793122	-1.062671	0.705380
H	1.857692	-1.554561	-1.635858

H	0.797045	-3.761962	-1.600838
H	1.983474	-5.721246	-0.608785
H	4.261668	-5.399013	0.332904
H	5.335153	-3.200276	0.297615
H	3.837878	-0.275781	-1.324878
H	6.302476	-1.197675	-0.974837
C	5.930515	0.811906	-0.316504
C	5.091848	1.732913	0.321443
C	7.087268	1.278716	-0.944520
C	5.408618	3.088023	0.333075
H	4.185016	1.382668	0.800637
C	7.408792	2.634861	-0.929362
H	7.740825	0.576474	-1.452086
C	6.569764	3.543293	-0.290013
H	4.748027	3.790276	0.829269
H	8.310066	2.980481	-1.423210
H	6.815177	4.599248	-0.280852
Si	-0.888519	-1.820346	2.081446
H	-2.091967	-1.356558	2.796041
C	0.614292	-1.898995	3.164153
C	0.687124	-1.143166	4.348356
C	1.688736	-2.744308	2.834328
C	1.802313	-1.228163	5.175444
H	-0.125794	-0.479109	4.620547
C	2.804494	-2.824014	3.663180
H	1.663346	-3.339556	1.927391
C	2.860293	-2.069163	4.832947
H	1.846473	-0.640416	6.085136
H	3.626928	-3.475348	3.392377
H	3.728576	-2.135529	5.479093
H	-1.117103	-3.074867	1.343327
O	-0.565336	-0.607324	0.848945
B	-1.601010	0.239932	-0.070304
C	-2.809336	-0.828122	-0.301364
C	-4.091217	-0.727355	0.241298
C	-2.590484	-1.973747	-1.072091
C	-5.091174	-1.668391	0.015010
C	-3.555645	-2.938041	-1.317237
C	-4.823018	-2.779484	-0.770784
C	-0.743951	0.630940	-1.417071
C	-1.259392	0.643232	-2.713633
C	0.582754	1.039253	-1.325396
C	-0.512692	1.016171	-3.827326
C	1.373244	1.397756	-2.405506

C	0.816170	1.387932	-3.676749
C	-1.983751	1.626787	0.713177
C	-1.499603	2.054497	1.945135
C	-2.833427	2.535967	0.080818
C	-1.831951	3.274847	2.524461
C	-3.193905	3.762525	0.617156
C	-2.685519	4.137506	1.855018
H	0.290807	-0.155835	0.933258
F	-6.303121	-1.516832	0.559855
F	-5.768743	-3.693680	-0.990240
F	-3.278738	-4.013287	-2.063492
F	-4.427141	0.298462	1.043857
F	-1.375822	-2.192318	-1.620482
F	1.191215	1.087961	-0.097286
F	2.664241	1.723131	-2.236611
F	1.549812	1.728261	-4.737309
F	-1.060919	1.005030	-5.045619
F	-2.528149	0.277346	-2.954140
F	-4.021198	4.582613	-0.039184
F	-3.364027	2.215735	-1.115755
F	-3.016009	5.314028	2.392543
F	-1.330640	3.619733	3.717338
F	-0.649518	1.281440	2.673664

$[Me_2NH_2]^+(C_6F_5)_3B\text{-}OH^-$

Sum of electronic and thermal Free Energies= -2420.367202 Hartree/Particle

B	-0.033332	0.134095	0.518446
C	-1.613864	0.588762	0.372996
C	-2.171464	0.771717	-0.893318
C	-2.510166	0.778964	1.417222
C	-3.498955	1.106742	-1.115542
C	-3.849149	1.113529	1.252049
C	-4.349647	1.276655	-0.030020
C	0.144589	-1.268598	-0.361508
C	-0.413063	-2.455980	0.111927
C	0.779443	-1.390449	-1.598197
C	-0.324511	-3.678799	-0.541672
C	0.880352	-2.590611	-2.296538
C	0.329592	-3.747464	-1.763338
C	1.051215	1.309624	0.096349
C	0.768537	2.625115	-0.261075
C	2.410710	1.034518	0.203377
C	1.751633	3.583259	-0.503789
C	3.426281	1.948393	-0.017593

C	3.090431	3.246032	-0.381158
F	1.510914	-2.642700	-3.476306
F	0.430350	-4.911147	-2.413582
F	-0.853862	-4.786809	0.003384
F	-1.088562	-2.474709	1.292558
F	1.341205	-0.324512	-2.194282
F	-4.651189	1.276506	2.312935
F	-5.633245	1.597689	-0.219780
F	-2.104160	0.649038	2.720013
F	-1.391387	0.647734	-1.985619
F	-3.967700	1.271692	-2.358442
F	2.821537	-0.226369	0.552157
F	4.715032	1.597435	0.123507
F	4.045533	4.155714	-0.600634
F	1.412816	4.833546	-0.842917
F	-0.501318	3.060142	-0.380542
O	0.315236	-0.194687	1.964306
H	1.245470	-1.219583	2.359452
H	-0.406376	0.023205	2.560983
H	2.395675	-2.279059	1.732816
N	2.008014	-1.988647	2.630533
C	1.353602	-3.144230	3.299726
H	0.908328	-2.797275	4.231814
H	0.567788	-3.529569	2.654109
H	2.088101	-3.921546	3.512750
C	3.080640	-1.344479	3.435247
H	3.529632	-0.555113	2.837662
H	2.633833	-0.918136	4.332748
H	3.835316	-2.080822	3.714313

Me_2NH

Sum of electronic and thermal Free Energies= -135.138900 Hartree/Particle

H	-0.000234	1.329011	0.517241
N	-0.000049	0.563942	-0.148655
C	1.215566	-0.222502	0.020295
H	1.283158	-0.965931	-0.780333
H	2.089768	0.428006	-0.061080
H	1.275338	-0.764987	0.981392
C	-1.215555	-0.222567	0.020307
H	-1.275366	-0.764830	0.981504
H	-2.089878	0.427712	-0.061563
H	-1.282503	-0.966158	-0.780188

$[Me_2NH_2]^+$

Sum of electronic and thermal Free Energies= -135.493828 Hartree/Particle

H	0.000018	1.159241	0.816065
N	0.000058	0.540855	0.000007
H	0.000041	1.159234	-0.816117
C	1.267963	-0.276169	-0.000002
H	1.276863	-0.896385	-0.894126
H	2.120956	0.400164	0.001905
H	1.275093	-0.899118	0.892237
C	-1.268050	-0.276171	-0.000002
H	-1.276605	-0.896720	0.893885
H	-2.120916	0.400308	-0.001327
H	-1.275332	-0.898668	-0.892545