Supporting Information

Silicon-Aryl Cooperative Activation of Ammonia

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Experimental

General procedures

All experiments were performed under a dry argon (≥99.996%) atmosphere using standard *Schlenk* techniques or in a glovebox (MBraun GmbH). Non-deuterated solvents used were distilled over sodium/benzophenone and stored over molecular sieve prior to use. Ammonia (99.98%) was purchased from Westfalen AG. Liquid Injection Field Desorption Ionization Mass Spectrometry (LIFDI-MS) was measured directly from an inert atmosphere glovebox with a Thermo Fisher Scientific Exactive Plus Orbitrap equipped with an ion source from Linden CMS.[1] NMR spectra were recorded on *Bruker* AV-400 or AV-500C spectrometers at ambient temperature (300 K). ^{1}H, ^{13}C, and ^{29}Si chemical shifts δ are reported in parts per million (ppm) relative to tetramethylsilane. $\delta(^{1}H)$ and $\delta(^{13}C)$ were referenced internally to the relevant residual solvent resonances. $\delta(^{29}Si)$ was referenced to the signal of tetramethylsilane (δ = 0 ppm) as external standard. For reported signals, the following abbreviations are used: s = singlet, d = doublet, hept = heptet, m = multiplet/signal overlap, br = broad signal, dd = doublet of doublets, dt = doublet of triplets. Melting Points (m.p.) were determined in sealed glass capillaries under an inert gas atmosphere using a Büchi B-540 melting point apparatus. Compound **1** was prepared according to literature procedures.[2]

3-(2,6-diisopropylphenyl)-5-(1,1,1,3,3,3-hexamethyl-2-(tri-p-tolylsilyl)trisilan-2-yl)-5a,9-diisopropyl-3,5,5a,8-tetrahydrobenzo[e]imidazo[1,2-a][1,3,4]azaphosphasilin-5-amine (**2**)

In a *J-Young* PTFE tube, IDippPSi(TMS)$_2$(SiTol$_3$) (**1**, 50 mg, 54.1 µmol) was dissolved in toluene and briefly immersed in liquid nitrogen until the solvent was frozen solid. The remaining argon atmosphere was removed *in vacuo* and ammonia (1 bar) was filled into the tube. While the solution was warmed to room temperature, its color changed from dark brown to yellow. The complete formation of **2** was confirmed *via* ^{31}P NMR. Crystals of compound **2** could be obtained from a saturated pentane solution (37.5 mg, 74%).

^{1}H NMR (500 MHz, C_6D_6) δ 7.89 (d, *J* = 8.0 Hz, 6H), 7.19 – 7.13 (m, 2H), 7.10 (d, *J* = 7.5 Hz, 6H), 7.03 (dd, *J* = 5.7, 3.5 Hz, 1H), 6.20 (dd, *J* = 2.2, 1.2 Hz, 1H), 6.09 (dd, *J* = 2.2, 1.1 Hz, 1H), 5.50 (dt, *J* = 10.0, 3.4 Hz, 1H), 5.40 (dt, *J* = 9.9, 1.8 Hz, 1H), 3.06 (hept, *J* = 6.8 Hz, 1H), 2.82 (hept, *J* = 6.9 Hz, 1H), 2.75 – 2.65 (m, 2H), 2.11 (s, 9H), 2.12 – 1.99 (m, 2H), 1.51 (d, *J* = 6.8 Hz, 3H), 1.43 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 6.9 Hz, 3H), 1.06 (d, *J* = 7.0 Hz, 3H), 1.05 (br, 2H), 1.03 (d, *J* = 7.0 Hz, 3H), 0.94 (dd, *J* = 9.3, 6.8 Hz, 6H), 0.82 (d, *J* = 6.9 Hz, 3H), 0.49 (d, *J* = 5.5 Hz, 18H).

^{13}C NMR (126 MHz, C_6D_6) δ 173.19 (d, J = 103.5 Hz), 147.58, 146.68, 138.80, 137.64, 136.07, 134.95, 133.90, 132.48, 130.32, 129.76, 128.82, 128.35, 124.75, 124.22, 120.64, 119.94 (d, J = 4.9 Hz), 118.87, 48.39 (d, J = 2.5 Hz), 31.37, 29.17, 28.81 (d, J = 7.0 Hz), 26.60, 24.78 (d, J = 6.5 Hz), 24.18, 24.04 (d, J = 3.5 Hz), 22.54, 21.53, 21.47, 21.44, 20.22, 4.87 (d, J = 5.5 Hz), 4.65 (d, J = 3.9 Hz).

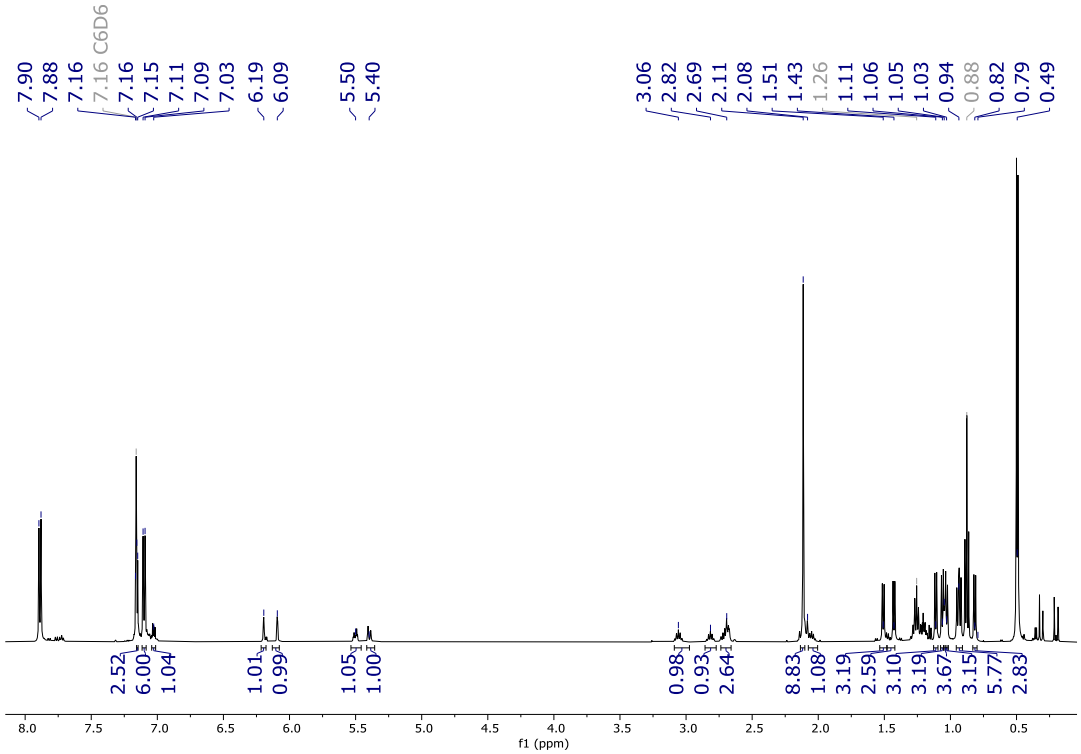
^{29}Si NMR (99 MHz, C_6D_6) δ 3.23 (d, *J* = 91.8 Hz, P-*Si*), -9.30 (d, *J* = 67.3 Hz, *TMS*), -10.35 (d, *J* = 9.6 Hz, *Si*Tol$_3$), -121.07 (d, *J* = 27.4 Hz, *Si*(TMS)$_2$(SiTol$_3$)).

^{31}P NMR (162 MHz, C_6D_6) δ -133.09.

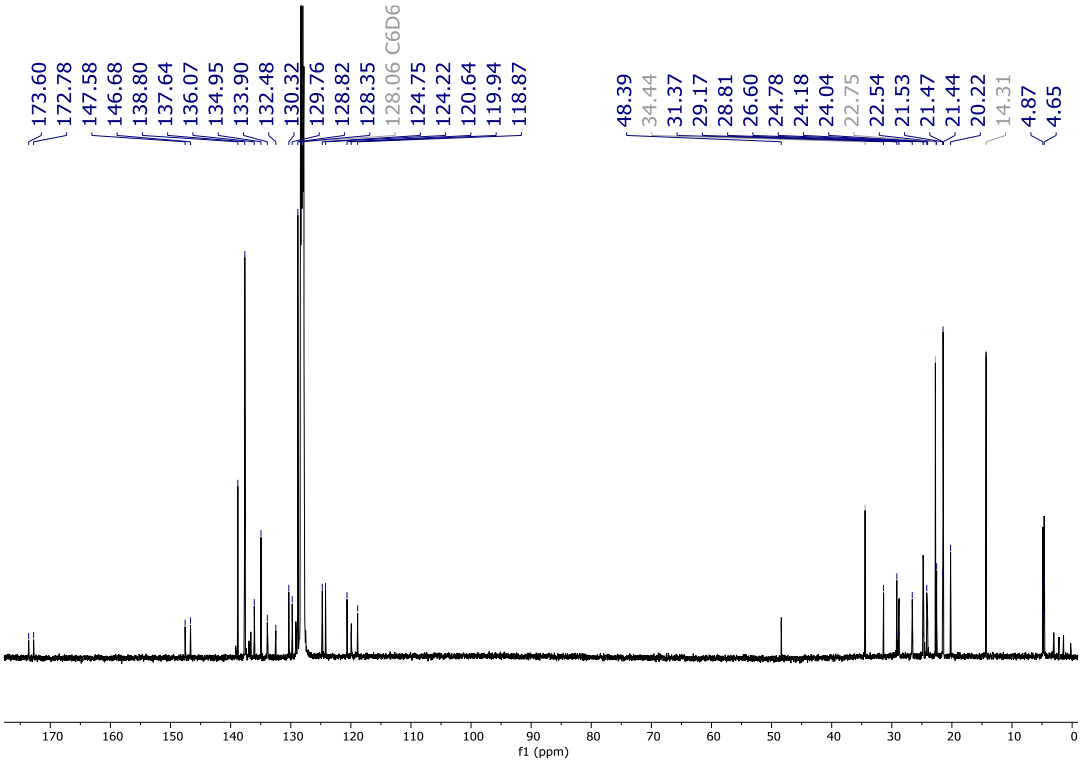
LIFDI-MS: calculated: 939.4780; found: 939.4768.

m.p.: 214.4 °C

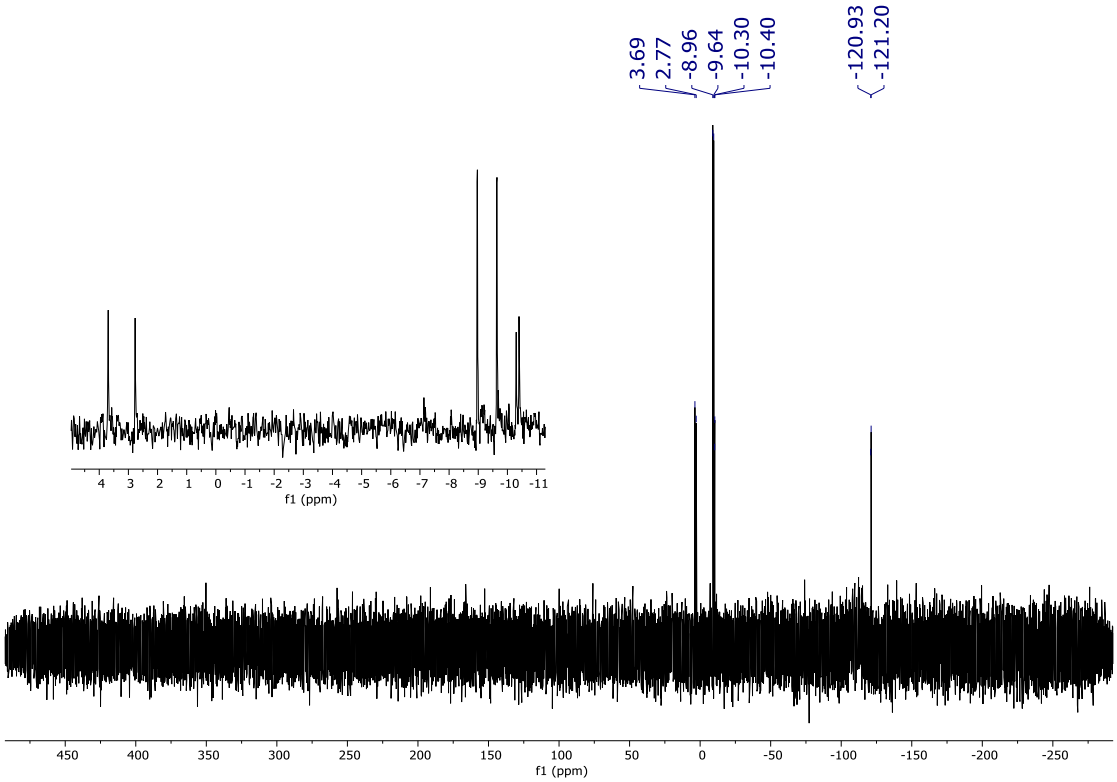
Spectra



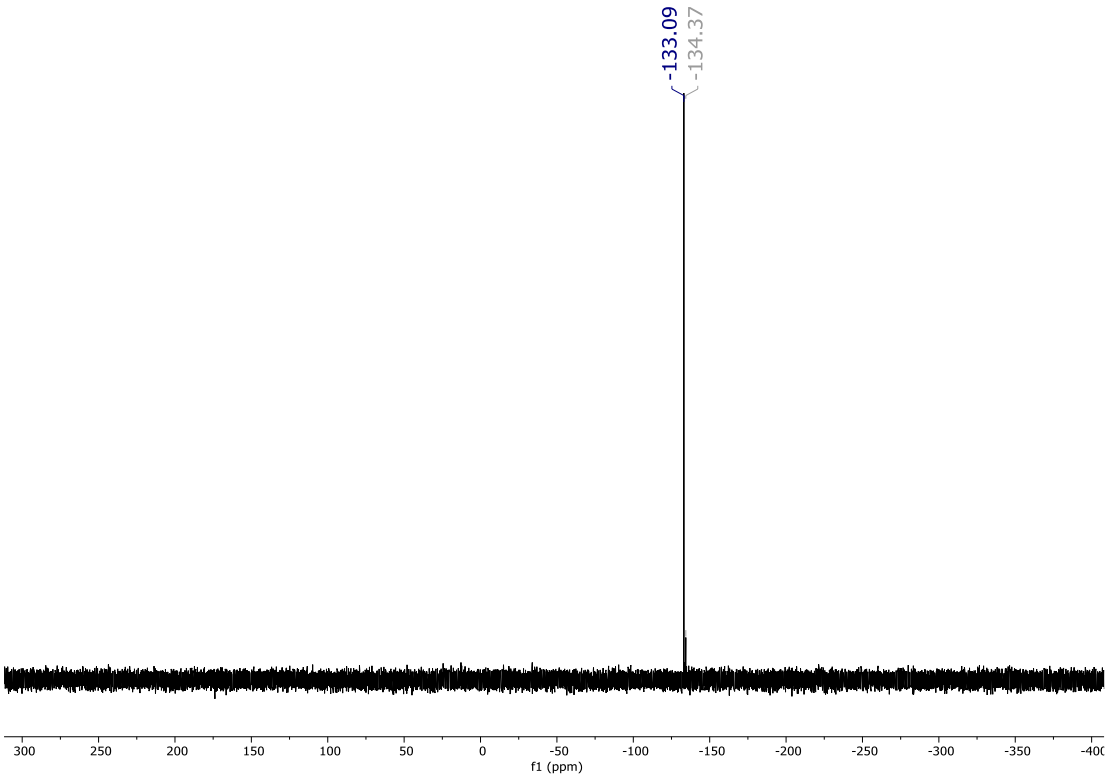
Supplementary Figure 1: ^{1}H NMR of **2**. Signals marked in grey correspond to co-crystallized pentane.



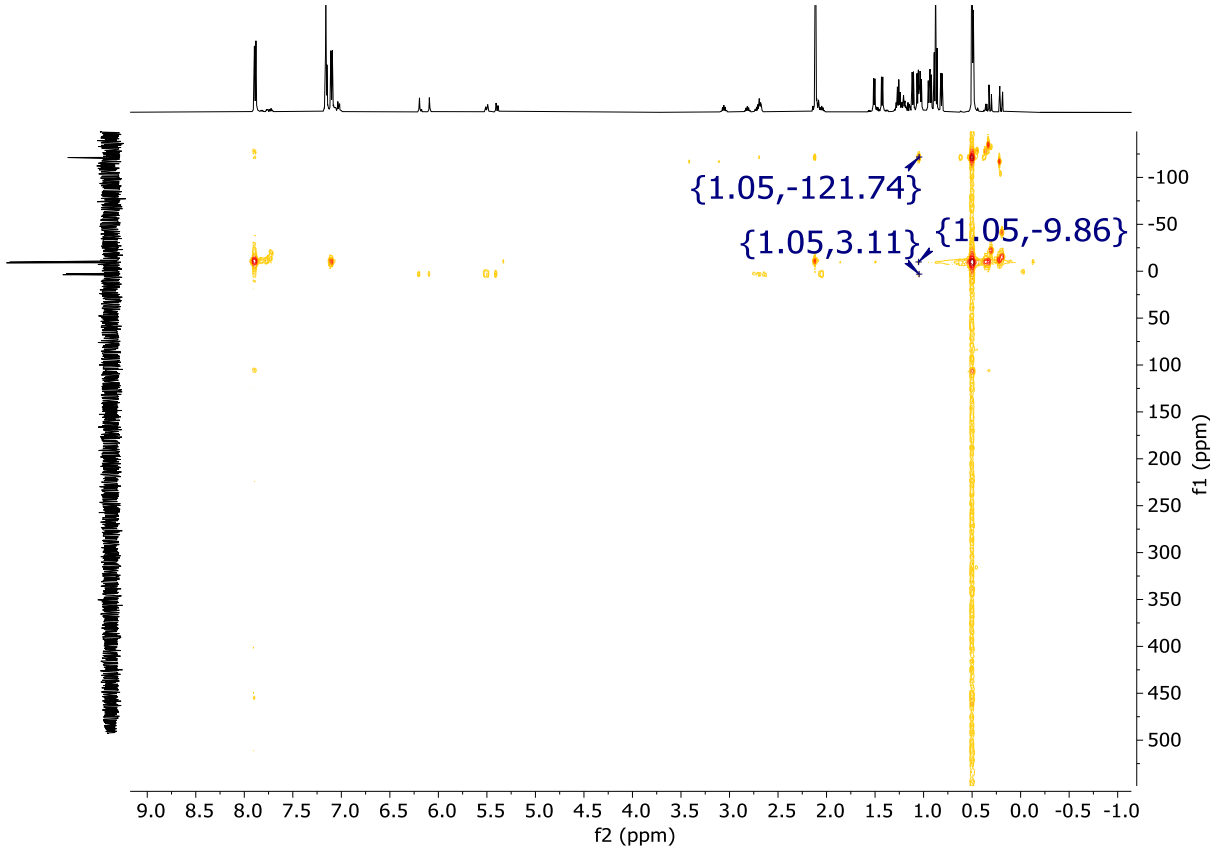
Supplementary Figure 2: ^{13}C NMR of **2**. Signals marked in grey correspond to co-crystallized pentane.



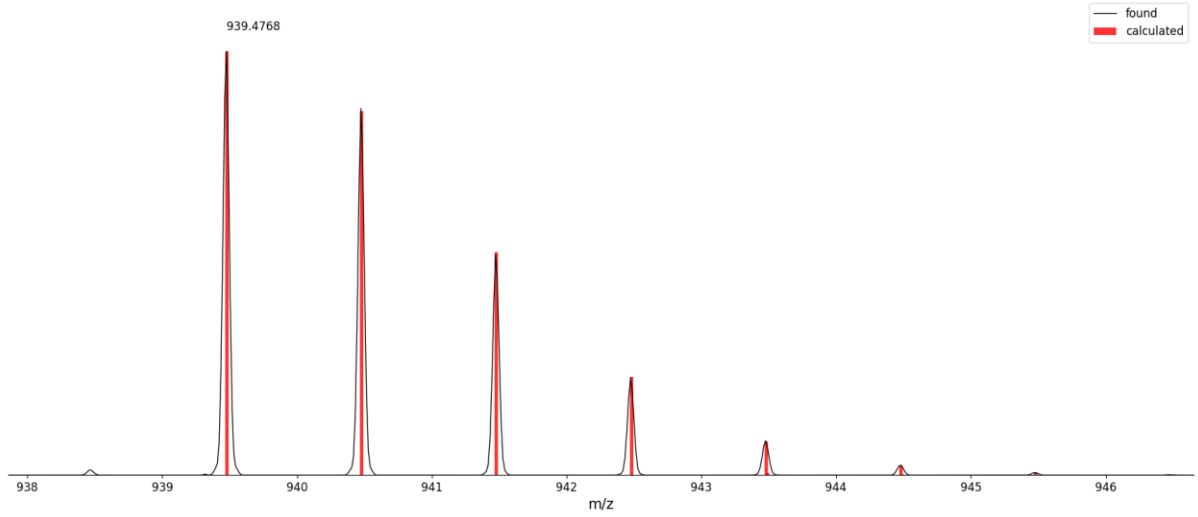
Supplementary Figure 3: ^{29}Si NMR of **2**.



Supplementary Figure 4: ^{31}P NMR of **2**. The signal in grey is IDippPH, a ubiquitous impurity when working with Dipp-NHCPs.



Supplementary Figure 5: SiH HMBC spectrum of **2**.



Supplementary Figure 6: LIFDI-MS spectrum of **2**.

Computational Details

Calculations were carried out using ORCA 5.0.4 software.[3]

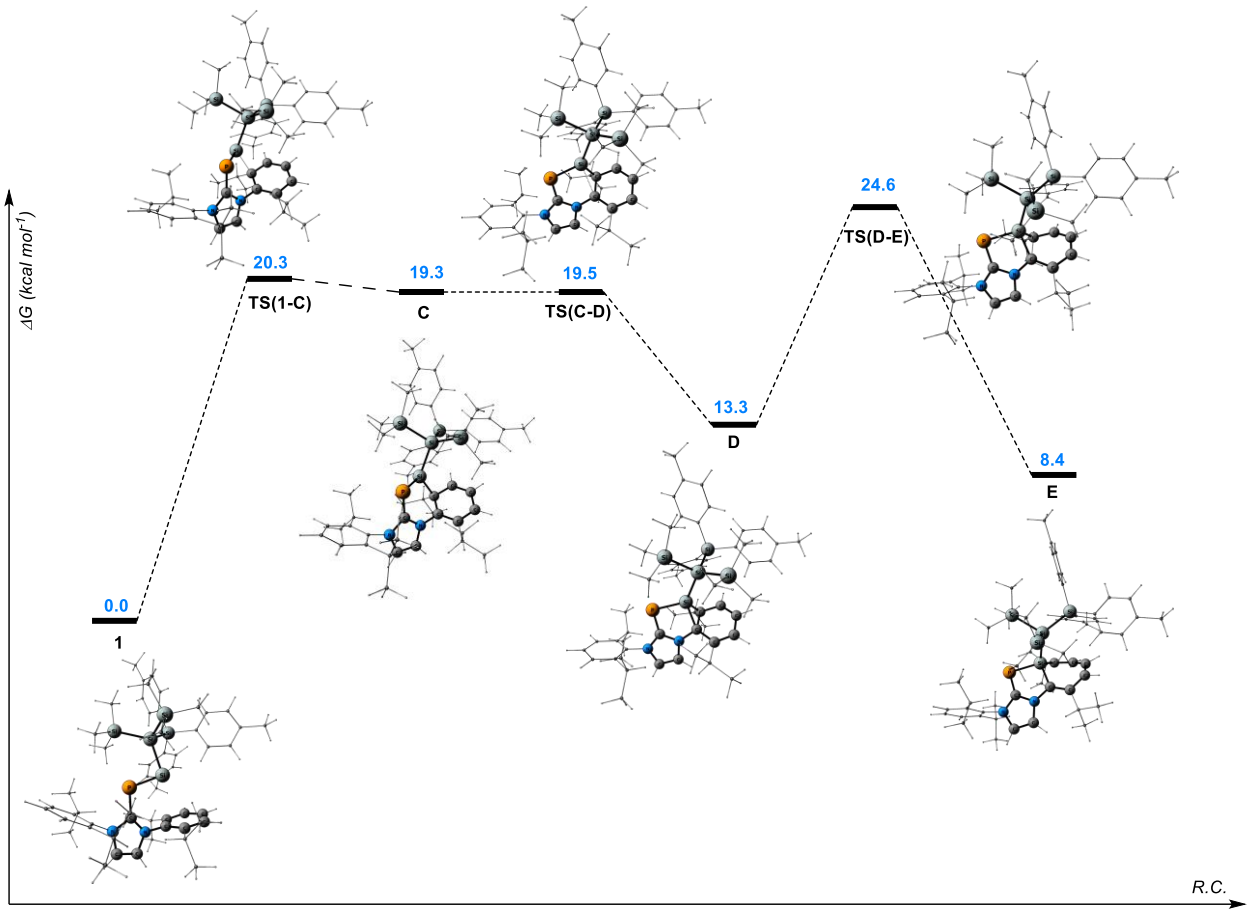
Geometry optimizations were carried using the r^{2}SCAN-3c composite method, utilizing the regularized and restored SCAN functional,[4, 5] geometrical counterpoise correction gCP,[6] the atom-pairwise dispersion correction based on tight binding partial charges (D4,[7-9] the def2-mTZVPP basis set and def2-mTZVPP/J auxiliary basis set.[10]

The optimized geometries were verified as minima or transition states by analytical frequency calculations. The transition states were additionally verified by IRC calculations. Single point calculations of the optimized geometries were carried out at the r^{2}SCAN-3c level in benzene using the SMD solvation module[11] to obtain electrostatic contribution and the cavity term to account for the solvent effects.

To get more accurate electronic energies for the mechanistic investigations, single point calculations of the r^{2}SCAN-3c optimized geometries were carried out using the PW6B95[12] functional, with D4 dispersion correction, the def2-QZVPP[13] basis set and def2/J[14] and def2-QZVPP/C[15] auxiliary basis sets. The method is denoted as PW6B95-D4(SMD=Benzene)/def2-QZVPP//r^{2}SCAN-3c. The summary of the thermochemistry results is presented in Supplementary Table 1.

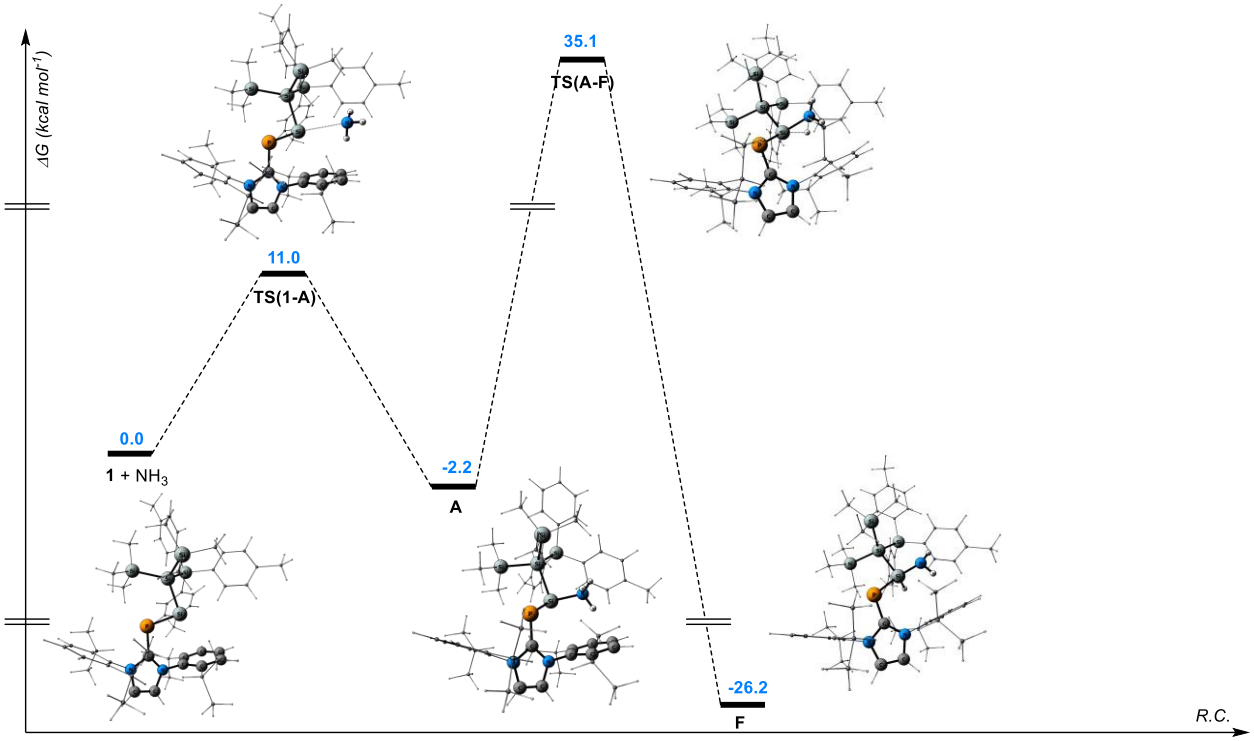
Supplementary Table 1: Calculated energies (Eh). E_{PW6B95} - electronic energy at the PW6B95-D4/def2-QZVPP//r^{2}SCAN-3c level; G-E_{el} - Gibbs energy minus the electronic energy at the r^{2}SCAN-3c// r^{2}SCAN-3c level; G_{cds} (cavity term) and G_{enp} (electrostatic contribution) at r^{2}SCAN-3c SMD=Benzene)// r^{2}SCAN-3c level; G_{conc} - concentration-induced free-energy shift (G_{conc} = RTln(24.5); G – free energy at the PW6B95-D4(SMD=Benzene)/def2-QZVPP//r^{2}SCAN-3c level, G = E_{PW6B95} + [G-E_{el}] + G_{cds} + G_{enp} + G_{conc}. Thermochemistry at 298.15 K.

Compound	ID	E_{PW6B95}	G-E_{el}	G_{cds}	G_{enp}	G_{conc}	G
NH_3	3755810	-56.65245	0.01638	-0.00500	0.00237	0.00302	-56.63568
1	3519997	-4007.10251	1.05124	-0.02633	-0.02620	0.00302	-4006.10077
TS(1-A)	3519955	-4063.75419	1.08593	-0.02749	-0.02623	0.00302	-4062.71897
A	3520171	-4063.77777	1.08904	-0.02758	-0.02674	0.00302	-4062.74003
TS(A-B)	3519949	-4063.75442	1.09113	-0.02534	-0.02551	0.00302	-4062.71112
B	3520170	-4063.75635	1.09098	-0.02581	-0.02555	0.00302	-4062.71371
TS(B-2)	3519725	-4063.74961	1.08816	-0.02520	-0.02506	0.00302	-4062.70870
2	3518893	-4063.80112	1.09138	-0.02377	-0.02489	0.00302	-4062.75537
TS(1-C)	3520303	-4007.07561	1.05237	-0.02201	-0.02625	0.00302	-4006.06848
C	3520751	-4007.07735	1.05216	-0.02179	-0.02606	0.00302	-4006.07003
TS(C-D)	3979989	-4007.07945	1.05337	-0.02116	-0.02544	0.00302	-4006.06966
D	3919971	-4007.09070	1.05402	-0.02103	-0.02492	0.00302	-4006.07960
TS(D-E)	3919973	-4007.06803	1.05392	-0.02167	-0.02582	0.00302	-4006.05857
E	3922447	-4007.09744	1.05451	-0.02161	-0.02590	0.00302	-4006.08742
TS(A-F)	3919972	-4063.71407	1.08275	-0.02544	-0.02670	0.00302	-4062.68044
F	3975127	-4063.81571	1.08678	-0.02589	-0.02642	0.00302	-4062.77822
G	4152498	-4120.43877	1.12460	-0.02931	-0.02495	0.00302	-4119.36541
TS(G-H)	4144987	-4120.41135	1.12410	-0.02756	-0.02531	0.00302	-4119.33710
H	4147236	-4120.47569	1.11953	-0.02669	-0.02406	0.00302	-4119.40389
I	4144972	-4120.41603	1.12303	-0.02775	-0.02392	0.00302	-4119.34164
TS(I-J)	4140701	-4120.40055	1.12399	-0.03002	-0.02421	0.00302	-4119.32778
J	4143801	-4120.45885	1.12545	-0.02685	-0.02338	0.00302	-4119.38061



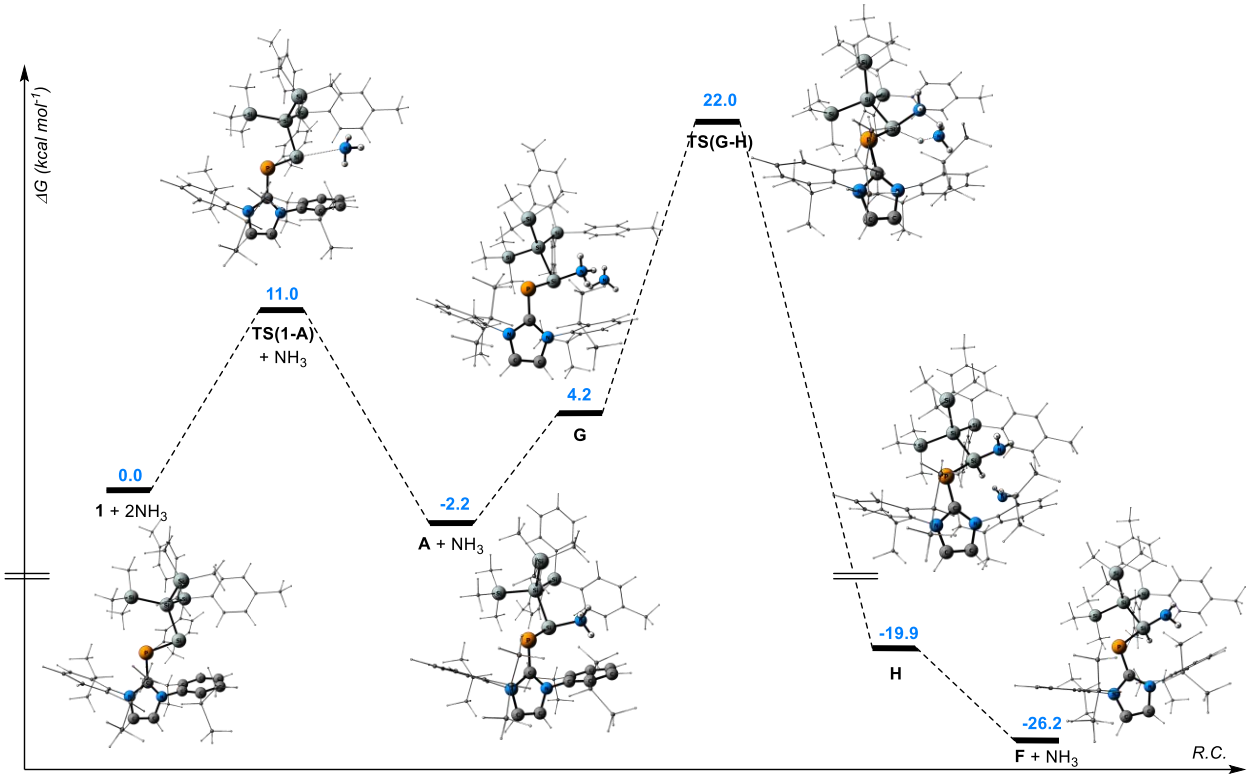
Supplementary Figure 7: Calculated free energy reaction coordinate diagram of the proposed mechanism for the conversion of **1** to the silepin **E** at the PW6B95-D4/def2-QZVPP(SMD = Benzene)//r^{2}SCAN-3c level of theory.

Supplementary Figure **7** describes the intermolecular insertion of the silylene into the C-C bond of the aryl substituent of the NHCP moiety. The first step is the formation of the Meisenheimer-type complex **C**, which rearranges to the formal product of [1+2] cycloaddition of the Si across the aromatic C-C bond **D**. The final step is the ring expansion to yield the final silepin product **E**, via the rate determining transition state **TS(D-E)** at 24.6 kcal mol^{-1}. **TS(D-E)** is by 7.2 kcal mol^{-1} higher than the rate determining transition state **TS(B-2)** that leads to the formation of **2**. In any case, the whole process is endergonic by 8.4 kcal mol^{-1} and thus the **E** would not be observed even with more favorable kinetics. In addition, the transition state **TS(1-C)**, which leads to the Meisenheimer-type complex **C**, is also higher than **TS(B-2)**. Thus, we rule out **C** as an intermediate in the formation of **2**.



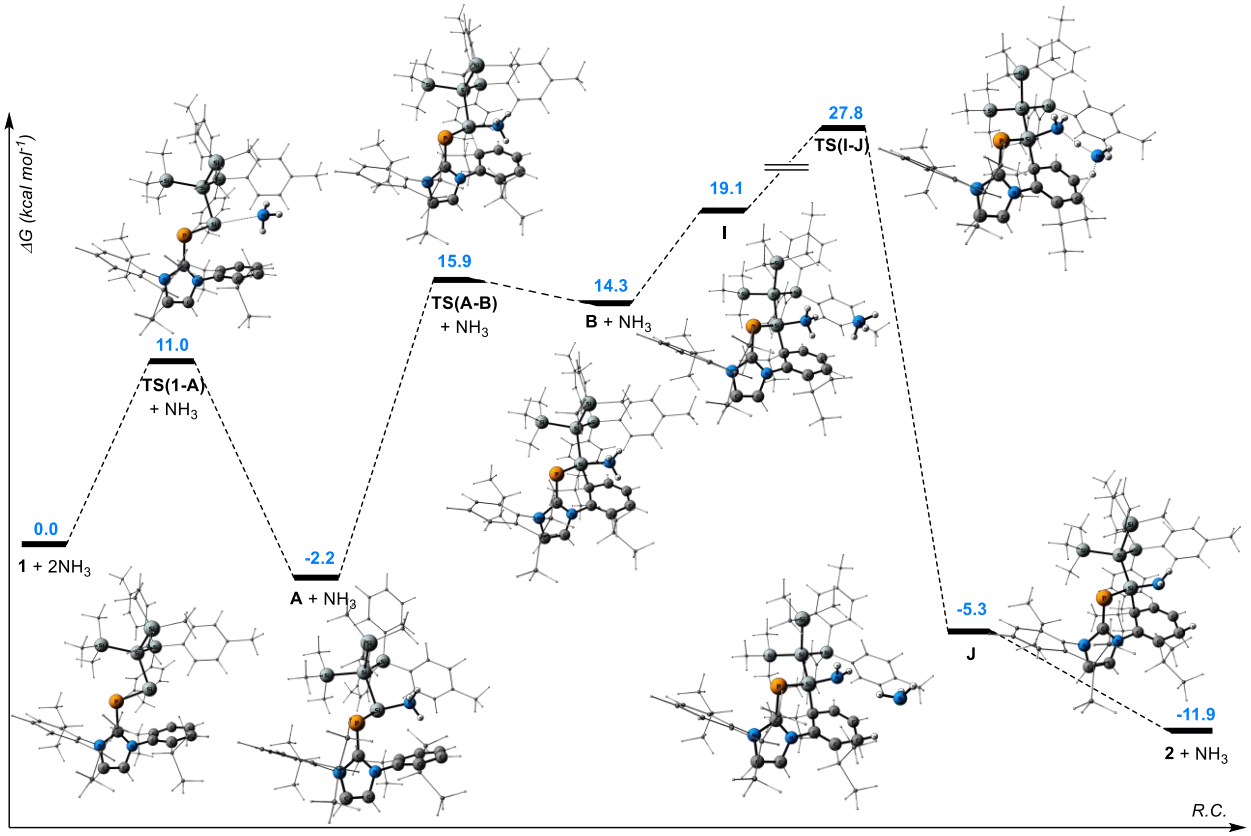
Supplementary Figure 8: Calculated free energy reaction coordinate diagram for 1,1-additon of ammonia at the Si center of **1** at the PW6B95-D4/def2-QZVPP(SMD = Benzene)//r²SCAN-3c level of theory.

Supplementary Figure **8** describes the oxidative addition of the silylene by insertion into the N-H bond of ammonia. Upon initial coordination of an ammonia molecule to the silylene center via **TS(1-A)** the resulting complex **A** undergoes the 1,1-addition to the form the product **F** in a very exergonic step. However, the barrier for this reaction **TS(A-F)** of 37.3 kcal mol^{-1} is infeasible.



Supplementary Figure 9: Calculated free energy reaction coordinate diagram for 1,1-additon of ammonia at the Si center of **1** via proton shuffling mechanism at the PW6B95-D4/def2-QZVPP(SMD = Benzene)//r^{2}SCAN-3c level of theory.

Supplementary Figure **9** describes the oxidative addition of the Si by two ammonia molecules. Upon formation of complex **A**, a second molecule of NH_3 can abstract a proton for the ammonia molecule that is coordinated to the silicon center, while simultaneously transferring a proton the silicon center. The rate determining transition state **TS(G-H)** at 22.0 kcal mol^{-1} is by 4.6 kcal mol^{-1} lower in energy than **TS(B-2)**. Therefore, the activation of ammonia via the mechanism presented in Fig. 2 of the main text, in which the single ammonia molecule is activated across the Si and the C centers is much more favorable.



Supplementary Figure 10: Calculated free energy reaction coordinate diagram for cooperative silylene-aryl activation of ammonia via proton shuffling mechanism at the PW6B95-D4/def2-QZVPP(SMD = Benzene)//r^{2}SCAN-3c level of theory.

Supplementary Figure **10** describes the ammonia activation across the Si center of the silylene and the C center of the aryl via a proton shuffling mechanism. Upon formation of complex **B**, a second molecule of NH_3 comes in. Via **TS(I-J)** a proton from the first ammonia molecule that is coordinated to the Si center is transferred to second ammonia molecule, while a proton from the second ammonia molecule is transferred to the C center. The rate determining transition state **TS(I-J)** at 27.8 kcal mol^{-1} is by 10.4 kcal mol^{-1} lower in energy than **TS(B-2)**. Therefore, the mechanism presented in Fig. 2 of the main text, in which the single ammonia molecule is activated across the Si and the C centers is much more favorable.

Cartesian coordinates and energies of the optimized geometries at the r^{2}SCAN-3c level

Calculated energies and coordinates of **1**

Electronic energy ... -4000.71363631 Eh
Total Enthalpy ... -3999.48791788 Eh
Final Gibbs free energy ... -3999.66239289 Eh

CARTESIAN COORDINATES (ANGSTROEM)

P	-0.697162	0.845006	0.261773
Si	0.221508	1.043881	-1.689356
Si	1.383547	-1.040523	-1.677125
Si	1.164175	-2.597273	0.095317
Si	0.953097	-2.112637	-3.745026
Si	3.603009	-0.199500	-1.786728
N	-2.796463	2.760232	0.131386
N	-0.905300	3.687177	0.640264
C	-3.057957	0.872668	-3.642785
H	-3.958890	0.510970	-4.150503
H	-2.541894	0.017096	-3.194222
H	-2.398815	1.302055	-4.404005
C	-3.377281	1.931188	-2.583569
H	-2.413282	2.323477	-2.236452
C	-4.107830	1.356968	-1.387362
C	-3.815318	1.764635	-0.078899
C	-1.471650	2.488759	0.309794
C	1.599561	-4.333456	-0.514929
C	0.613279	-5.306269	-0.720104
H	-0.421285	-5.081523	-0.468520
C	0.929709	-6.561993	-1.231684
H	0.139925	-7.295791	-1.379853
C	2.245761	-6.898273	-1.550566
C	2.587803	-8.241855	-2.134553
H	2.677894	-8.179992	-3.226225
H	1.815811	-8.983037	-1.908615
H	3.543576	-8.611556	-1.749860
C	-5.129532	0.421050	-1.549398
H	-5.388243	0.079859	-2.546796
C	-5.819787	-0.081710	-0.453700
H	-6.614153	-0.807976	-0.603811
C	-5.495118	0.331223	0.830149
H	-6.030843	-0.080853	1.680344
C	-4.480121	1.263766	1.048270
C	-4.105990	1.659717	2.464049
H	-3.381151	2.480328	2.416204
C	-5.315965	2.174776	3.253705
H	-5.809013	3.003257	2.734031
H	-4.997321	2.527904	4.240309
H	-6.059123	1.385877	3.410472
C	-3.428403	0.484500	3.183666
H	-4.120363	-0.358769	3.285675
H	-3.111965	0.787466	4.188514
H	-2.552844	0.131122	2.629056
C	-4.177854	3.093446	-3.190266
H	-3.633505	3.531701	-4.033821
H	-4.358230	3.883362	-2.453161
H	-5.151342	2.744421	-3.553946
C	-3.050674	4.105187	0.347704
H	-4.043776	4.516834	0.258581
C	-1.869089	4.683672	0.670612
H	-1.624935	5.702931	0.923232
C	0.462899	3.863812	1.052721
C	1.374427	4.434833	0.153945
C	2.683876	4.615003	0.602774
H	3.422301	5.047060	-0.065113
C	3.062169	4.229448	1.880667
H	4.090051	4.367251	2.203803
C	2.136109	3.662342	2.745440
H	2.444316	3.371762	3.745304
C	0.811388	3.468973	2.353749
C	-0.203351	2.915535	3.337856
H	-1.091685	2.602770	2.779980
C	0.301233	1.675148	4.080266
H	0.596485	0.890820	3.377907
H	-0.495650	1.276052	4.716464
H	1.153891	1.902573	4.729407
C	-0.632509	4.015888	4.320973
H	-1.035224	4.887743	3.793919
H	0.219212	4.351534	4.923571
H	-1.404165	3.638800	5.001646
C	0.972440	4.872536	-1.242228
H	0.034794	4.363979	-1.498783
C	2.001147	4.472707	-2.305416
H	1.605349	4.695089	-3.301790
H	2.213120	3.400668	-2.262485
H	2.940803	5.024158	-2.192848
C	0.734790	6.390910	-1.278726
H	1.660391	6.928441	-1.042574
H	-0.023849	6.705056	-0.555005
H	0.405154	6.702094	-2.275966
C	0.708572	-0.819893	-5.105265
H	0.479582	-1.316025	-6.057015
H	1.596079	-0.197124	-5.251886
H	-0.124537	-0.151940	-4.859775
C	2.354285	-3.276869	-4.248514
H	2.135141	-3.732204	-5.222695
H	2.474118	-4.081672	-3.515101
H	3.311833	-2.751460	-4.331092
C	-0.636565	-3.136948	-3.676493
H	-1.515463	-2.507578	-3.496604
H	-0.594141	-3.900423	-2.892636
H	-0.785099	-3.648377	-4.636135
C	3.888305	1.199199	-0.542510
H	4.761017	1.792613	-0.844649
H	4.078636	0.801484	0.459139
H	3.029895	1.875631	-0.468737
C	3.891082	0.524189	-3.513271
H	4.876314	1.005550	-3.556162
H	3.134552	1.278181	-3.758653

H	3.860403	-0.247190	-4.289873
C	4.928666	-1.509002	-1.465581
H	4.846390	-2.355413	-2.155562
H	4.854084	-1.888523	-0.439903
H	5.925677	-1.066650	-1.587713
C	-0.602938	-2.677756	0.753117
C	-1.709571	-2.487030	-0.082404
H	-1.555259	-2.201348	-1.120214
C	-3.008368	-2.630329	0.391646
H	-3.847985	-2.461127	-0.279401
C	-3.249340	-2.967830	1.724771
C	-4.652758	-3.175747	2.225763
H	-5.369079	-2.582078	1.649607
H	-4.746708	-2.906807	3.282870
H	-4.947517	-4.228455	2.130838
C	-2.151531	-3.134634	2.572154
H	-2.316745	-3.379876	3.619765
C	-0.852464	-2.993663	2.094808
H	-0.017207	-3.125919	2.780055
C	2.323366	-2.155551	1.518061
C	2.443154	-0.823396	1.938030
H	1.879339	-0.044265	1.425673
C	3.270410	-0.471660	2.998006
H	3.343284	0.573468	3.295073
C	4.014306	-1.436859	3.681157
C	3.892758	-2.767395	3.275464
H	4.454545	-3.539060	3.798260
C	3.063930	-3.120210	2.214199
H	2.992028	-4.166207	1.923903
C	4.940524	-1.048112	4.801383
H	5.082177	-1.872635	5.506392
H	4.556287	-0.184768	5.353523
H	5.929361	-0.774472	4.412549
C	2.921170	-4.683124	-0.830919
H	3.719718	-3.960155	-0.682105
C	3.239373	-5.939059	-1.331668
H	4.275437	-6.179319	-1.563233

Calculated energies and coordinates of **TS[1-A]**

Electronic energy ... -4057.25049648 Eh
Total Enthalpy ... -4055.98548895 Eh
Final Gibbs free energy ... -4056.16457146 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.206789	9.257034	9.531505
Si	-1.417474	10.302546	11.270695
Si	-0.385266	9.248172	13.175517
P	-2.151866	9.579011	14.441484
Si	-3.737436	9.927626	10.911178
Si	-1.063664	12.649281	11.266174
N	-2.915405	8.505622	16.879019
N	-0.915283	7.789666	16.441301
N	2.030988	11.293416	13.324057
C	-3.077104	10.410957	4.128630
H	-4.097578	10.753037	4.340327
H	-3.149317	9.522485	3.495135
H	-2.581649	11.201973	3.556213
C	-2.338294	10.116192	5.405490
C	-2.143774	8.806799	5.844810
H	-2.513188	7.980872	5.240334
C	-1.487761	8.540798	7.044610
H	-1.356245	7.508030	7.360152
C	-1.005497	9.576054	7.852910
C	-1.906494	8.602327	15.947349
C	-4.133899	9.272733	16.861371
C	-4.159727	10.479442	17.570770
C	-2.935405	11.045117	18.265398
H	-2.163304	10.268321	18.291704
C	-3.225535	11.441983	19.718013
H	-3.919419	12.287234	19.775700
H	-2.298278	11.745873	20.215422
H	-3.661124	10.609506	20.280678
C	-6.472407	10.722928	16.899144
H	-7.395050	11.296175	16.909107
C	-6.413104	9.524646	16.196988
H	-7.288993	9.180044	15.657988
C	-5.240992	8.772202	16.158397
C	-5.358253	11.196482	17.573830
H	-5.412390	12.142987	18.103424
C	-2.368823	12.229218	17.467376
H	-2.107985	11.926973	16.447444
H	-1.470301	12.621051	17.957207
H	-3.101867	13.041397	17.404578
C	-2.540195	7.684563	17.927893
H	-3.192119	7.506272	18.768577
C	-1.291153	7.241149	17.656842
H	-0.629894	6.595110	18.212358
C	-0.101599	7.387865	9.816439
C	-0.882145	6.707941	10.755499
H	-1.597282	7.259198	11.362241
C	-0.765087	5.332338	10.939389
H	-1.394930	4.834250	11.673546
C	0.147777	4.584574	10.196440
C	0.940772	5.256711	9.260789
H	1.667187	4.697001	8.674477
C	0.816727	6.627937	9.075161
H	1.458660	7.123614	8.348760
C	0.266177	3.095538	10.378905
H	-0.256908	2.560134	9.577019
H	-0.171017	2.775183	11.329338
H	1.312307	2.773494	10.354872
C	-1.851387	11.156623	6.203279
H	-1.992879	12.187364	5.883453
C	-1.207021	10.890071	7.403199
H	-0.868017	11.725297	8.013935
C	1.597052	9.828555	9.470837
C	2.123177	10.629002	8.450974
H	1.486991	10.936504	7.623916
C	3.455975	11.030121	8.459005
H	3.834595	11.650443	7.648993
C	4.318595	10.642441	9.485330
C	5.750398	11.103902	9.513778
H	5.851408	12.025683	10.100366
H	6.121398	11.314780	8.506472

H	6.402412	10.352870	9.970378
C	3.807121	9.823142	10.495930
H	4.464044	9.488462	11.297283
C	2.474969	9.423946	10.488653
H	2.107805	8.781055	11.288790
C	-4.781939	10.904932	12.151506
H	-4.559073	11.976619	12.126797
H	-4.607225	10.554656	13.174348
H	-5.846840	10.779938	11.914019
C	-4.194318	8.100463	11.109407
H	-5.282420	7.985803	11.022153
H	-3.892372	7.715145	12.090047
H	-3.730758	7.481945	10.333303
C	-4.284875	10.425496	9.170221
H	-3.774627	9.834556	8.402720
H	-4.088349	11.481125	8.960092
H	-5.365229	10.256192	9.071588
C	-2.383473	13.557549	10.252102
H	-3.393566	13.379674	10.634102
H	-2.368802	13.255511	9.199484
H	-2.194802	14.638163	10.293824
C	-1.182956	13.246652	13.052117
H	-0.368942	12.809289	13.640153
H	-2.128982	12.937570	13.511076
H	-1.112574	14.340467	13.105232
C	0.600875	13.175018	10.540291
H	0.750008	14.248610	10.713761
H	0.641378	13.001874	9.459835
H	1.441241	12.636434	10.984636
C	0.730960	6.569204	15.088531
C	-0.177041	5.393728	14.749483
H	0.198838	5.027944	13.783788
C	0.028058	4.266114	15.775749
H	-0.352703	4.563137	16.759575
H	1.086795	4.010097	15.883346
H	-0.517220	3.367436	15.466040
C	-1.671112	5.668914	14.551950
H	-2.125989	4.804124	14.056033
H	-1.841585	6.551751	13.927768
H	-2.198698	5.806060	15.501324
C	2.031371	6.525643	14.579321
H	2.304911	5.707901	13.917141
C	2.961344	7.508345	14.879258
H	3.961883	7.451921	14.459830
C	2.619943	8.559281	15.720361
H	2.271060	10.480395	13.882466
H	3.365265	9.307472	15.977081
C	1.333886	8.660695	16.248627
C	0.990727	9.789534	17.204130
H	-0.088403	9.774600	17.385806
C	1.320009	11.171479	16.631561
H	2.395755	11.291368	16.457618
H	1.015843	11.948549	17.340816
H	0.794714	11.340436	15.687093
C	1.692053	9.566432	18.552832
H	2.781213	9.600707	18.436861
H	1.430852	8.592468	18.980136
H	1.402425	10.345282	19.266971
C	0.408329	7.662672	15.903320
C	-5.160411	7.467040	15.389296
H	-4.140962	7.391326	14.989367
C	-6.115249	7.416996	14.194738
H	-7.160552	7.330327	14.512404
H	-5.888059	6.540619	13.579517
H	-6.012226	8.305695	13.565406
C	-5.408721	6.265821	16.315214
H	-4.690064	6.228650	17.139417
H	-5.323117	5.329596	15.752367
H	-6.416062	6.316573	16.744513
H	2.337462	11.083106	12.379085
H	2.588795	12.073747	13.656937

Calculated energies and coordinates of **A**

Electronic energy ... -4057.27477323 Eh
Total Enthalpy ... -4056.00789667 Eh
Final Gibbs free energy ... -4056.18573410 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.507124	9.036752	9.307383
Si	-1.752095	9.886711	11.137602
Si	-0.619042	8.798916	12.959630
P	-1.854156	9.803818	14.582256
Si	-3.952743	9.019889	11.146018
Si	-1.877299	12.253183	11.037670
N	-2.387551	8.908225	17.142771
N	-0.408059	8.213863	16.565220
N	0.986416	10.059094	12.932240
C	-1.183179	12.119219	3.937463
H	-0.244548	12.561613	3.590787
H	-1.930781	12.914039	4.016197
H	-1.524658	11.423248	3.161116
C	-1.001590	11.405827	5.249566
C	0.220557	10.818318	5.585115
H	1.058341	10.898024	4.895098
C	0.381035	10.133465	6.785321
H	1.345499	9.683120	7.011062
C	-0.671770	10.016666	7.703345
C	-1.496834	8.918755	16.082862
C	-3.673888	9.542825	17.125801
C	-3.768202	10.879315	17.533616
C	-2.552435	11.697738	17.920886
H	-1.660262	11.091435	17.731729
C	-2.575673	12.048088	19.414650
H	-3.435992	12.682424	19.655799
H	-1.667103	12.593029	19.694598
H	-2.640820	11.146665	20.033508
C	-6.159325	10.730849	17.187276
H	-7.140116	11.197274	17.214874
C	-6.032397	9.415678	16.757259
H	-6.915812	8.869679	16.442098
C	-4.785226	8.794519	16.710212
C	-5.038986	11.456176	17.564340
H	-5.150148	12.490454	17.877905
C	-2.431288	12.956031	17.051659

H	-2.410132	12.685156	15.991465
H	-1.506962	13.493356	17.291821
H	-3.267739	13.643088	17.220553
C	-1.847730	8.257511	18.240138
H	-2.391902	8.161983	19.166438
C	-0.618737	7.823505	17.884548
H	0.126677	7.273239	18.436982
C	-0.979741	7.244929	8.936827
C	-1.269408	6.831137	7.629553
H	-1.226311	7.551854	6.815795
C	-1.622645	5.514844	7.349513
H	-1.849653	5.226476	6.325001
C	-1.693680	4.557615	8.363020
C	-1.412058	4.964090	9.669492
H	-1.479863	4.241758	10.481146
C	-1.067057	6.280667	9.952670
H	-0.886539	6.570860	10.988736
C	-2.043325	3.126966	8.055451
H	-1.138990	2.539562	7.852809
H	-2.685277	3.054580	7.172465
H	-2.559477	2.653715	8.896223
C	-2.058346	11.286007	6.154790
H	-3.020735	11.735569	5.917866
C	-1.893720	10.605226	7.355834
H	-2.733498	10.528659	8.042159
C	1.321881	9.080718	9.817326
C	2.075877	10.261390	9.704033
H	1.645202	11.127396	9.207640
C	3.366411	10.356265	10.216401
H	3.920804	11.286751	10.108161
C	3.963562	9.269051	10.864275
C	5.348059	9.383818	11.441941
H	5.756331	8.401184	11.695293
H	5.344454	9.991697	12.355710
H	6.033909	9.866111	10.737705
C	3.230518	8.086397	10.963426
H	3.677865	7.220646	11.447122
C	1.936488	7.992932	10.454240
H	1.399881	7.053487	10.552039
C	-5.036667	10.057041	12.297820
H	-5.105576	11.099503	11.968967
H	-4.631544	10.051528	13.316559
H	-6.055290	9.648115	12.324337
C	-3.971964	7.237695	11.769269
H	-5.007278	6.895194	11.892634
H	-3.466325	7.158392	12.738533
H	-3.472946	6.566747	11.063523
C	-4.739679	9.026100	9.423876
H	-4.136644	8.452316	8.710629
H	-4.860956	10.042241	9.032048
H	-5.735483	8.566749	9.467363
C	-3.263140	12.899206	9.917515
H	-4.235623	12.461866	10.165498
H	-3.054468	12.692567	8.863237
H	-3.347822	13.987397	10.034438
C	-2.185007	12.970886	12.761087
H	-1.381724	12.718838	13.462468
H	-3.111233	12.582391	13.197538
H	-2.261414	14.064359	12.700901
C	-0.271969	13.013234	10.375567
H	-0.329166	14.108134	10.421212
H	-0.117442	12.728602	9.328337
H	0.610896	12.699927	10.944420
C	1.236139	7.047688	15.162228
C	0.440046	5.758295	14.991885
H	0.674736	5.424262	13.971667
C	0.999661	4.708804	15.971182
H	0.798061	5.007478	17.006817
H	2.081469	4.583737	15.860714
H	0.518049	3.739439	15.802575
C	-1.086748	5.800307	15.094937
H	-1.483550	4.850514	14.718876
H	-1.505845	6.606562	14.485999
H	-1.430108	5.910967	16.128475
C	2.503438	7.073965	14.566255
H	2.797124	6.239143	13.934827
C	3.376229	8.134149	14.751797
H	4.348954	8.126660	14.267673
C	3.009241	9.204796	15.560035
H	1.696761	9.731237	13.585590
H	3.704809	10.024167	15.719910
C	1.753586	9.235906	16.171178
C	1.385842	10.409121	17.061899
H	0.408654	10.208995	17.511213
C	1.256437	11.711146	16.260436
H	2.186783	11.948066	15.729931
H	1.032513	12.546825	16.932647
H	0.436070	11.632241	15.537500
C	2.391151	10.561813	18.211815
H	3.384429	10.842708	17.845249
H	2.492131	9.628705	18.776032
H	2.057696	11.345373	18.900526
C	0.877634	8.158086	15.940606
C	-4.637204	7.362181	16.235774
H	-3.616344	7.248424	15.852396
C	-5.589067	7.021125	15.085718
H	-6.630086	6.956748	15.421925
H	-5.321888	6.047461	14.662248
H	-5.524304	7.766718	14.288636
C	-4.829728	6.377966	17.399571
H	-4.110955	6.556226	18.205459
H	-4.700153	5.346602	17.052567
H	-5.838311	6.474099	17.818476
H	1.407762	10.103929	12.002576
H	0.704317	10.994351	13.215223

Calculated energies and coordinates of **TS[A-B]**

Electronic energy ... -4057.25832664 Eh
Total Enthalpy ... -4055.99342011 Eh
Final Gibbs free energy ... -4056.16719886 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.144050	9.119059	9.456292
Si	-1.455516	10.226803	11.095015

Si	-0.773214	9.220743	13.185789
P	-2.233062	10.024160	14.675684
Si	-3.773219	9.808650	10.798564
Si	-1.101506	12.578634	11.114495
N	-2.862078	8.557147	16.962029
N	-0.884876	7.999762	16.233397
N	0.801050	10.392835	13.504503
C	-2.326367	9.859399	3.673379
H	-1.903831	9.125285	2.981220
H	-2.116378	10.860763	3.285358
H	-3.415573	9.728291	3.668299
C	-1.775944	9.683615	5.062219
C	-1.317185	8.440770	5.503014
H	-1.333011	7.593486	4.820472
C	-0.840384	8.269641	6.799141
H	-0.491505	7.287630	7.111186
C	-0.807690	9.336683	7.705857
C	-1.953058	8.817392	15.959075
C	-4.062150	9.307794	17.195604
C	-3.978315	10.443720	18.011220
C	-2.660811	10.951988	18.565278
H	-1.854616	10.322652	18.172524
C	-2.624723	10.851664	20.096065
H	-3.390214	11.488789	20.553027
H	-1.648690	11.174055	20.475476
H	-2.800350	9.823670	20.430327
C	-6.373818	10.690723	17.771951
H	-7.287684	11.230641	18.003764
C	-6.421752	9.581180	16.935754
H	-7.372859	9.274334	16.513337
C	-5.265328	8.867892	16.623178
C	-5.165007	11.122687	18.295927
H	-5.138126	12.004776	18.929594
C	-2.384740	12.385761	18.093197
H	-2.402501	12.439106	16.999913
H	-1.399047	12.714030	18.440807
H	-3.128467	13.087191	18.487117
C	-2.346879	7.623810	17.850074
H	-2.899922	7.306479	18.719887
C	-1.130445	7.260933	17.384277
H	-0.412794	6.544818	17.752552
C	-0.090870	7.267461	9.821006
C	-1.294945	6.563906	9.960133
H	-2.238775	7.094987	9.857432
C	-1.315818	5.197513	10.210900
H	-2.268907	4.682620	10.313695
C	-0.125906	4.476210	10.341367
C	1.078701	5.164428	10.182775
H	2.018127	4.620909	10.262712
C	1.096405	6.532226	9.923847
H	2.053862	7.031695	9.793785
C	-0.138917	3.009136	10.671247
H	0.682819	2.482010	10.176885
H	-1.080593	2.540442	10.371349
H	-0.021788	2.856099	11.751399
C	-1.739131	10.754328	5.959607
H	-2.092073	11.733307	5.640925
C	-1.270702	10.579534	7.255611
H	-1.278193	11.425637	7.938466
C	1.609030	9.818249	9.535291
C	2.116601	10.661867	8.539987
H	1.526132	10.853786	7.646484
C	3.362120	11.269800	8.673879
H	3.725621	11.925791	7.885423
C	4.152603	11.057855	9.804900
C	5.506839	11.698350	9.937915
H	5.751920	11.897769	10.985400
H	5.557137	12.641480	9.386210
H	6.288644	11.040829	9.537820
C	3.662036	10.201287	10.795250
H	4.262806	10.003878	11.681695
C	2.418994	9.593146	10.659245
H	2.084061	8.911847	11.441368
C	-4.777209	11.214628	11.563806
H	-4.576926	12.179795	11.086902
H	-4.561153	11.303443	12.634360
H	-5.847933	11.001487	11.450200
C	-4.336639	8.232804	11.673101
H	-5.401463	8.064302	11.467145
H	-4.212427	8.361135	12.753610
H	-3.786546	7.335383	11.376434
C	-4.226477	9.686096	8.967483
H	-3.693375	8.875949	8.458231
H	-3.989067	10.610171	8.429961
H	-5.304007	9.502270	8.868545
C	-1.851069	13.497000	9.631625
H	-2.835435	13.110566	9.347894
H	-1.198890	13.444876	8.753319
H	-1.968566	14.557497	9.888742
C	-1.884882	13.311508	12.672687
H	-1.570183	12.795114	13.586992
H	-2.977171	13.255107	12.642633
H	-1.602157	14.368631	12.759418
C	0.736517	13.050694	11.149886
H	0.822286	14.128035	10.957450
H	1.321511	12.526704	10.387342
H	1.208951	12.868095	12.121388
C	0.337560	7.497199	14.135303
C	-0.456907	6.215092	13.773267
H	-0.307976	6.106233	12.690173
C	0.182125	5.002124	14.464569
H	0.089111	5.086093	15.554276
H	1.247580	4.921340	14.227048
H	-0.320953	4.078583	14.155193
C	-1.965811	6.208671	14.010978
H	-2.413052	5.368192	13.467341
H	-2.433301	7.127834	13.643475
H	-2.219909	6.087313	15.070288
C	1.690887	7.439255	13.573115
H	1.796862	6.937716	12.613405
C	2.786713	7.974625	14.188879
H	3.755961	7.899825	13.698234
C	2.698086	8.604776	15.450491
H	1.405862	9.999276	14.236465
H	3.577606	9.038546	15.909701
C	1.468679	8.592333	16.123502

C	1.341154	9.325557	17.452623
H	0.479593	8.926434	17.997914
C	1.056213	10.814512	17.193465
H	1.897456	11.276113	16.661221
H	0.919396	11.352078	18.139525
H	0.148318	10.944166	16.590924
C	2.560692	9.154684	18.362878
H	3.442581	9.666427	17.964016
H	2.814665	8.097854	18.494064
H	2.352918	9.585531	19.348498
C	0.357974	7.990483	15.516403
C	-5.299482	7.658975	15.708536
H	-4.339049	7.629698	15.178877
C	-6.403354	7.743991	14.651383
H	-7.398982	7.619780	15.092309
H	-6.269222	6.944377	13.916063
H	-6.374322	8.700610	14.120249
C	-5.440480	6.358905	16.515763
H	-4.613225	6.226646	17.219012
H	-5.450708	5.494338	15.842722
H	-6.377113	6.361987	17.085605
H	1.370351	10.548780	12.671342
H	0.450266	11.290140	13.832336

Calculated energies and coordinates of **B**

Electronic energy ... -4057.25784946 Eh
Total Enthalpy ... -4055.99211103 Eh
Final Gibbs free energy ... -4056.16687333 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.037509	9.062789	9.460539
Si	-1.374912	10.120677	11.116259
Si	-0.773453	9.303674	13.304887
P	-2.285449	10.102018	14.724401
Si	-3.694415	9.731555	10.770581
Si	-1.067441	12.485255	11.108760
N	-2.916330	8.597611	16.992181
N	-0.927153	8.080510	16.255155
N	0.794264	10.448704	13.575155
C	-2.496816	9.940341	3.810562
H	-2.228898	9.140168	3.114696
H	-2.185992	10.894982	3.375321
H	-3.590946	9.957190	3.888767
C	-1.870764	9.725144	5.161029
C	-1.524671	8.446254	5.600050
H	-1.683946	7.594818	4.941615
C	-0.977901	8.243187	6.863834
H	-0.718742	7.233238	7.173253
C	-0.760456	9.313860	7.739239
C	-2.005169	8.887832	16.002201
C	-4.119564	9.338410	17.240579
C	-4.043241	10.448329	18.091823
C	-2.731991	10.936285	18.677874
H	-1.924384	10.300834	18.298872
C	-2.729768	10.824355	20.208027
H	-3.493853	11.470623	20.654257
H	-1.756786	11.127347	20.610131
H	-2.929252	9.796817	20.530048
C	-6.434504	10.711041	17.828466
H	-7.349681	11.247018	18.064136
C	-6.475046	9.626422	16.959729
H	-7.421814	9.334576	16.517550
C	-5.317062	8.918909	16.640801
C	-5.231593	11.122770	18.381022
H	-5.209821	11.985291	19.041233
C	-2.430259	12.370667	18.222833
H	-2.431555	12.435794	17.130015
H	-1.445356	12.682753	18.587247
H	-3.171419	13.077449	18.612229
C	-2.390723	7.651119	17.860722
H	-2.940374	7.311778	18.724392
C	-1.170477	7.310546	17.386194
H	-0.450510	6.586628	17.733448
C	0.032872	7.210536	9.798533
C	-1.162583	6.488272	9.916550
H	-2.113904	7.003555	9.798740
C	-1.164932	5.121920	10.169243
H	-2.110818	4.590992	10.255160
C	0.034293	4.422117	10.326653
C	1.230218	5.130223	10.190402
H	2.176776	4.603908	10.294896
C	1.230298	6.496481	9.926204
H	2.181018	7.014403	9.819982
C	0.040074	2.957042	10.664395
H	0.877204	2.440521	10.185025
H	-0.889512	2.471374	10.354169
H	0.144382	2.813469	11.747028
C	-1.643477	10.800347	6.024941
H	-1.900545	11.808582	5.705783
C	-1.105545	10.594577	7.288207
H	-0.957355	11.449450	7.943387
C	1.698882	9.802024	9.508717
C	2.205407	10.587585	8.466453
H	1.622229	10.718497	7.557766
C	3.444347	11.214836	8.571702
H	3.806894	11.824913	7.746847
C	4.229416	11.079070	9.717700
C	5.576407	11.739699	9.821314
H	5.800688	12.026558	10.853082
H	5.631331	12.634460	9.194669
H	6.369599	11.057174	9.491848
C	3.740987	10.277585	10.754044
H	4.337449	10.137892	11.654178
C	2.504431	9.652220	10.648286
H	2.171588	9.015241	11.467605
C	-4.702300	11.134837	11.534778
H	-4.480424	12.108612	11.086251
H	-4.518452	11.197681	12.613213
H	-5.770875	10.933942	11.384154
C	-4.296362	8.148819	11.602845
H	-5.342784	7.968302	11.325380
H	-4.249966	8.275849	12.689074
H	-3.715309	7.259416	11.343006
C	-4.107043	9.639871	8.928780

H	-3.592689	8.813789	8.426150
H	-3.828448	10.556366	8.398693
H	-5.188178	9.492944	8.809646
C	-1.925891	13.345003	9.647826
H	-2.832792	12.826872	9.321577
H	-1.258911	13.434011	8.783950
H	-2.208767	14.361880	9.947220
C	-1.805240	13.235286	12.681266
H	-1.402984	12.801354	13.603404
H	-2.890030	13.099197	12.724116
H	-1.597544	14.313194	12.693538
C	0.751691	13.017659	11.050184
H	0.787919	14.103656	10.893106
H	1.305721	12.541558	10.234813
H	1.294991	12.817323	11.980263
C	0.160582	7.665344	14.046165
C	-0.610806	6.346997	13.729722
H	-0.517482	6.238786	12.639536
C	0.086128	5.149164	14.382372
H	0.063636	5.239606	15.475351
H	1.135309	5.082508	14.078427
H	-0.422392	4.217210	14.108855
C	-2.105684	6.317416	14.047685
H	-2.579162	5.483009	13.516725
H	-2.601129	7.239305	13.728670
H	-2.298122	6.175096	15.117346
C	1.533600	7.559996	13.449825
H	1.592369	7.066265	12.483035
C	2.661780	8.009748	14.061051
H	3.615159	7.891580	13.546361
C	2.643775	8.617602	15.344464
H	1.418287	10.058099	14.303328
H	3.559304	8.981136	15.791990
C	1.441990	8.594287	16.070662
C	1.388989	9.263354	17.439529
H	0.579223	8.813984	18.023514
C	1.043088	10.753104	17.268844
H	1.842010	11.266055	16.718597
H	0.937694	11.242625	18.244737
H	0.104084	10.882008	16.716431
C	2.670602	9.095361	18.259408
H	3.506352	9.655820	17.827950
H	2.967332	8.043625	18.323227
H	2.514975	9.474097	19.275753
C	0.285524	8.066723	15.490869
C	-5.342849	7.735048	15.694021
H	-4.376803	7.719479	15.175233
C	-6.433412	7.848374	14.626181
H	-7.435674	7.727025	15.052426
H	-6.299078	7.059752	13.879021
H	-6.388267	8.813834	14.111895
C	-5.488622	6.413887	16.464919
H	-4.666484	6.265838	17.171176
H	-5.488662	5.568010	15.768462
H	-6.430521	6.397841	17.025766
H	1.349445	10.572223	12.726884
H	0.469397	11.361545	13.887240

Calculated energies and coordinates of **TS[B-2]**

Electronic energy ... -4057.25284936 Eh
Total Enthalpy ... -4055.99202728 Eh
Final Gibbs free energy ... -4056.16469054 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.000836	9.003656	9.479549
Si	-1.329327	10.032833	11.169607
Si	-0.602708	9.505913	13.406687
P	-2.249158	10.153861	14.768986
Si	-3.660625	9.667213	10.836354
Si	-1.121708	12.405737	11.006393
N	-2.950561	8.517744	16.931499
N	-0.947010	8.049582	16.212843
N	0.846914	10.677243	13.704912
C	-2.632387	10.100343	3.947158
H	-3.662201	10.442043	4.108447
H	-2.674966	9.207503	3.317136
H	-2.111468	10.888156	3.393792
C	-1.956067	9.814988	5.259612
C	-1.836448	8.512614	5.744826
H	-2.211368	7.684077	5.147629
C	-1.242729	8.255871	6.977840
H	-1.159685	7.227038	7.320170
C	-0.750090	9.294384	7.775815
C	-2.017075	8.873822	15.986763
C	-4.146815	9.258289	17.213019
C	-4.062419	10.321926	18.121276
C	-2.751061	10.761180	18.744613
H	-1.948302	10.132135	18.345040
C	-2.767586	10.576312	20.267656
H	-3.526464	11.212284	20.736867
H	-1.794390	10.846407	20.692125
H	-2.984414	9.537776	20.539319
C	-6.447369	10.632463	17.851151
H	-7.356818	11.169484	18.105758
C	-6.495656	9.593411	16.929244
H	-7.442992	9.337334	16.466681
C	-5.344771	8.885988	16.584435
C	-5.243719	10.997788	18.434083
H	-5.215905	11.824962	19.137794
C	-2.422503	12.210945	18.362427
H	-2.394332	12.323459	17.273993
H	-1.444060	12.493286	18.765941
H	-3.165860	12.908007	18.764822
C	-2.445737	7.506768	17.742137
H	-3.013744	7.111521	18.569127
C	-1.210372	7.204095	17.278935
H	-0.485968	6.476841	17.609610
C	0.081371	7.151328	9.815427
C	-1.099714	6.403100	9.911550
H	-2.057943	6.891067	9.745053
C	-1.080045	5.049826	10.227277
H	-2.015892	4.499637	10.301386
C	0.127175	4.390617	10.471668
C	1.310107	5.125402	10.363201

H	2.262781	4.633019	10.548118
C	1.289148	6.476899	10.034524
H	2.229140	7.019685	9.961931
C	0.157646	2.929074	10.824616
H	-0.812777	2.589115	11.197236
H	0.911256	2.724193	11.591442
H	0.408958	2.320092	9.947467
C	-1.441751	10.855959	6.039187
H	-1.505110	11.879568	5.674758
C	-0.854833	10.598122	7.270137
H	-0.455431	11.430056	7.846823
C	1.740221	9.735762	9.492897
C	2.331463	10.300637	8.356381
H	1.802698	10.283420	7.406525
C	3.593868	10.885244	8.414743
H	4.025781	11.316280	7.513840
C	4.319024	10.923697	9.606715
C	5.665381	11.590036	9.677108
H	5.565805	12.633002	10.002466
H	6.158696	11.595904	8.700934
H	6.321874	11.086139	10.392972
C	3.748695	10.333008	10.738112
H	4.301216	10.318555	11.676223
C	2.486220	9.756402	10.679856
H	2.094589	9.274609	11.575206
C	-4.664402	10.962616	11.778189
H	-4.471750	11.987060	11.447972
H	-4.457087	10.901633	12.852369
H	-5.732411	10.759552	11.623905
C	-4.318525	8.006561	11.450690
H	-5.357675	7.899561	11.112986
H	-4.319450	7.989737	12.544015
H	-3.756057	7.137140	11.100791
C	-4.066835	9.805671	8.995396
H	-3.630532	8.984642	8.416793
H	-3.698381	10.738405	8.557066
H	-5.156103	9.773661	8.863921
C	-2.220494	13.134798	9.645958
H	-3.282919	12.984602	9.858783
H	-2.022167	12.712854	8.657432
H	-2.042087	14.216580	9.593835
C	-1.676236	13.248841	12.609172
H	-1.001767	13.069389	13.452487
H	-2.671718	12.921657	12.924796
H	-1.712233	14.333690	12.445306
C	0.649233	12.971933	10.648094
H	0.663124	14.065894	10.559397
H	1.044208	12.549567	9.718282
H	1.353514	12.699889	11.441737
C	0.244293	7.861152	14.018399
C	-0.470105	6.536762	13.615237
H	-0.286498	6.457145	12.535285
C	0.186091	5.325391	14.284154
H	0.026884	5.346149	15.369136
H	1.265721	5.302206	14.108648
H	-0.251231	4.397405	13.897247
C	-1.987139	6.477602	13.798759
H	-2.395784	5.656173	13.198327
H	-2.469418	7.403134	13.471188
H	-2.274043	6.295864	14.841032
C	1.674139	7.783411	13.513039
H	1.836330	7.180917	12.623402
C	2.699289	8.388819	14.140713
H	3.704134	8.304911	13.728492
C	2.482264	9.215673	15.312464
H	1.664866	10.239143	14.493018
H	3.360904	9.570763	15.845508
C	1.321907	8.868076	16.099309
C	1.227098	9.409676	17.512973
H	0.278136	9.084636	17.952857
C	1.213513	10.945685	17.499953
H	2.152634	11.347639	17.105148
H	1.079878	11.331806	18.517463
H	0.388016	11.318753	16.882182
C	2.349665	8.871469	18.409140
H	3.331345	9.224088	18.077459
H	2.367641	7.776471	18.399307
H	2.203925	9.205312	19.442833
C	0.293534	8.187426	15.509774
C	-5.384663	7.743628	15.588201
H	-4.402343	7.702867	15.101099
C	-6.433694	7.946164	14.492192
H	-7.453547	7.879659	14.886904
H	-6.329492	7.164098	13.733598
H	-6.313489	8.916407	13.999223
C	-5.618946	6.403976	16.304149
H	-4.842898	6.200220	17.047833
H	-5.616438	5.581353	15.580474
H	-6.588391	6.408190	16.816222
H	1.365401	10.884289	12.851583
H	0.492403	11.559030	14.069284

Calculated energies and coordinates of **2**

Electronic energy ... -4057.29904654 Eh
Total Enthalpy ... -4056.03316380 Eh
Final Gibbs free energy ... -4056.20766428 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.023032	9.015486	9.522998
Si	-1.373038	9.970634	11.207997
Si	-0.608879	9.718950	13.470897
P	-2.288236	10.296510	14.844037
Si	-3.673914	9.474351	10.820846
Si	-1.313135	12.346326	10.943594
N	-2.984489	8.642385	16.977173
N	-1.006685	8.127333	16.221141
N	0.693967	10.859552	13.746070
C	-2.550328	10.083375	3.953400
H	-3.591747	10.395947	4.099062
H	-2.558445	9.194843	3.315777
H	-2.041114	10.889244	3.415590
C	-1.890049	9.804751	5.275480
C	-1.779150	8.504867	5.769406
H	-2.147145	7.673430	5.171823

C	-1.202432	8.254458	7.011511
H	-1.124362	7.226873	7.358705
C	-0.717733	9.295951	7.810387
C	-2.057700	8.991354	16.016507
C	-4.155830	9.411044	17.282561
C	-4.029738	10.467311	18.194450
C	-2.697597	10.862981	18.803002
H	-1.917559	10.224207	18.374214
C	-2.693148	10.644111	20.321835
H	-3.432217	11.284038	20.816650
H	-1.708418	10.886183	20.736655
H	-2.926444	9.604284	20.574503
C	-6.408788	10.843998	17.958550
H	-7.299461	11.404650	18.228171
C	-6.498289	9.811744	17.032282
H	-7.458388	9.583896	16.580932
C	-5.371604	9.075739	16.667879
C	-5.187594	11.173211	18.527085
H	-5.128121	11.995946	19.234079
C	-2.340144	12.312333	18.447523
H	-2.329827	12.448668	17.361576
H	-1.347341	12.560964	18.838254
H	-3.057215	13.018369	18.880570
C	-2.502465	7.599420	17.757920
H	-3.074853	7.196339	18.578014
C	-1.284772	7.267096	17.275208
H	-0.589083	6.498624	17.572873
C	0.198033	7.157742	9.802654
C	-0.936677	6.340435	9.894059
H	-1.924520	6.779275	9.768782
C	-0.833533	4.978083	10.150531
H	-1.734906	4.371989	10.216561
C	0.414472	4.378746	10.337417
C	1.551761	5.182047	10.228013
H	2.535342	4.734438	10.356447
C	1.446586	6.543225	9.960879
H	2.352591	7.140813	9.881162
C	0.533734	2.917960	10.674048
H	1.390488	2.461797	10.168356
H	-0.367580	2.367419	10.390221
H	0.681042	2.781213	11.752645
C	-1.381818	10.848392	6.055080
H	-1.436493	11.869962	5.683644
C	-0.809554	10.596523	7.294484
H	-0.410907	11.430522	7.868468
C	1.741885	9.800826	9.524431
C	2.367590	10.208224	8.339455
H	1.862537	10.068262	7.386882
C	3.630866	10.793556	8.353312
H	4.088580	11.101142	7.415335
C	4.322366	10.990108	9.549380
C	5.670099	11.657340	9.570069
H	5.572849	12.720936	9.820543
H	6.163056	11.591534	8.596013
H	6.326405	11.205105	10.320221
C	3.714647	10.564290	10.733827
H	4.236133	10.687486	11.681575
C	2.451560	9.987285	10.718437
H	2.022958	9.655622	11.660061
C	-4.751797	10.716404	11.752977
H	-4.613141	11.746684	11.413983
H	-4.538091	10.679212	12.827288
H	-5.807209	10.453927	11.601610
C	-4.305459	7.775717	11.368457
H	-5.282890	7.608836	10.897187
H	-4.448065	7.747717	12.451840
H	-3.652196	6.942474	11.096920
C	-4.039796	9.610834	8.970802
H	-3.612116	8.771136	8.413093
H	-3.644694	10.527356	8.523407
H	-5.127222	9.597679	8.821305
C	-2.448937	12.973557	9.560171
H	-3.503214	12.778037	9.777163
H	-2.228043	12.536565	8.582849
H	-2.324350	14.061207	9.479217
C	-1.907243	13.206355	12.519678
H	-1.212574	13.061530	13.352032
H	-2.887223	12.845768	12.847717
H	-1.989284	14.284458	12.329972
C	0.422167	13.000697	10.562300
H	0.372721	14.091791	10.452905
H	0.845238	12.585690	9.641675
H	1.131012	12.779520	11.366268
C	0.129761	7.964660	14.024928
C	-0.658250	6.698905	13.567024
H	-0.562257	6.704210	12.472701
C	0.010770	5.420427	14.083691
H	-0.037207	5.374083	15.179353
H	1.063565	5.364078	13.790508
H	-0.506176	4.537907	13.689321
C	-2.156280	6.653867	13.871217
H	-2.628241	5.888299	13.244870
H	-2.637830	7.610998	13.656001
H	-2.359453	6.390886	14.915185
C	1.494265	7.883460	13.418111
H	1.526293	7.523267	12.391507
C	2.625658	8.189225	14.046766
H	3.575739	8.098413	13.522112
C	2.665119	8.666723	15.460789
H	3.030808	9.706751	15.493734
H	3.410867	8.085649	16.026553
C	1.336585	8.596595	16.164416
C	1.295547	9.144140	17.580306
H	0.404761	8.761191	18.088499
C	1.149144	10.675952	17.523701
H	2.005125	11.139242	17.020768
H	1.090709	11.087557	18.538552
H	0.242085	10.955972	16.976990
C	2.508953	8.741175	18.424691
H	3.431242	9.201538	18.054502
H	2.650399	7.654578	18.433102
H	2.369512	9.072769	19.458986
C	0.236822	8.184698	15.507934
C	-5.456304	7.940013	15.667309
H	-4.473218	7.853706	15.189389
C	-6.483070	8.194669	14.560942

H	-7.509100	8.181610	14.944867
H	-6.413288	7.405957	13.804955
H	-6.307991	9.156185	14.068164
C	-5.759545	6.611981	16.379136
H	-5.002600	6.375716	17.133057
H	-5.783981	5.789448	15.655712
H	-6.733964	6.659018	16.879429
H	1.267952	11.174306	12.976502
H	0.459685	11.634772	14.350064

Calculated energies and coordinates of **TS[1-C]**

Electronic energy ... -4000.69175512 Eh
Total Enthalpy ... -3999.46776129 Eh
Final Gibbs free energy ... -3999.63938528 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.132206	9.116613	9.511298
Si	-1.559287	9.947832	11.212405
Si	-1.761486	8.459467	13.075547
P	-2.508318	9.784968	14.671364
Si	-3.789884	9.864307	10.380893
Si	-1.089802	12.220102	11.725122
N	-2.781675	8.647831	17.231135
N	-0.953928	7.979989	16.246087
C	-2.665963	10.201038	3.926327
H	-3.671550	10.616581	4.066424
H	-2.765272	9.289656	3.329991
H	-2.090663	10.930590	3.347608
C	-2.016377	9.920992	5.253724
C	-2.000386	8.634866	5.794354
H	-2.438249	7.813034	5.231604
C	-1.424823	8.386510	7.037551
H	-1.412457	7.368186	7.420941
C	-0.851616	9.416543	7.792155
C	-2.096223	8.728378	16.043530
C	-4.016982	9.326267	17.493719
C	-3.957607	10.626872	18.013698
C	-2.642977	11.330724	18.292308
H	-1.826100	10.681008	17.958795
C	-2.459286	11.570354	19.797541
H	-3.229634	12.245395	20.186563
H	-1.482340	12.025199	19.994623
H	-2.521794	10.632099	20.359063
C	-6.379030	10.640707	18.014679
H	-7.311311	11.159375	18.219526
C	-6.405180	9.356128	17.488901
H	-7.359623	8.880225	17.282805
C	-5.222258	8.668431	17.215745
C	-5.168532	11.268983	18.274004
H	-5.162873	12.277635	18.677305
C	-2.530259	12.641111	17.502487
H	-2.661868	12.458719	16.431340
H	-1.542143	13.088582	17.656670
H	-3.281779	13.369498	17.826609
C	-2.074859	7.894938	18.150440
H	-2.457720	7.706871	19.141321
C	-0.941739	7.474139	17.538626
H	-0.148773	6.831146	17.886519
C	0.149816	7.261950	9.720507
C	-0.899261	6.394194	10.055296
H	-1.904959	6.786210	10.181880
C	-0.679391	5.034770	10.251023
H	-1.515193	4.387239	10.509557
C	0.601935	4.490317	10.136530
C	1.650814	5.347232	9.793310
H	2.656908	4.945495	9.691369
C	1.428507	6.704970	9.585353
H	2.269164	7.347259	9.330910
C	0.848847	3.032533	10.412665
H	1.726611	2.666745	9.872058
H	-0.012553	2.421382	10.126789
H	1.028082	2.866544	11.482601
C	-1.426441	10.951543	5.992235
H	-1.416005	11.961621	5.587171
C	-0.861530	10.704853	7.236612
H	-0.415578	11.531483	7.785639
C	1.544968	9.976692	9.587680
C	2.296130	10.243566	8.435689
H	1.893189	9.986005	7.458514
C	3.553028	10.836134	8.516027
H	4.113970	11.032311	7.604562
C	4.107268	11.183438	9.749637
C	5.448771	11.858511	9.836451
H	5.331696	12.946127	9.920474
H	6.053467	11.660051	8.947053
H	6.007205	11.522480	10.715683
C	3.366565	10.911418	10.903096
H	3.777944	11.169129	11.877736
C	2.110312	10.323499	10.821102
H	1.558577	10.124912	11.737259
C	-5.040726	10.183076	11.760135
H	-4.882126	11.140209	12.265081
H	-4.987484	9.401124	12.524628
H	-6.054404	10.181875	11.339092
C	-4.225580	8.175123	9.651579
H	-5.260542	8.198925	9.286952
H	-4.159360	7.383965	10.407061
H	-3.581930	7.911989	8.806034
C	-4.041603	11.154651	9.023609
H	-3.411792	10.940956	8.154075
H	-3.808143	12.167515	9.368207
H	-5.089697	11.144769	8.698072
C	-0.532017	13.194103	10.202617
H	-1.293001	13.183416	9.414654
H	0.398398	12.786517	9.791257
H	-0.348360	14.240451	10.478542
C	-2.653617	13.038562	12.403546
H	-3.011734	12.521130	13.300401
H	-3.464997	13.050469	11.668787
H	-2.431823	14.078127	12.676711
C	0.239820	12.368429	13.058553
H	0.156723	13.339524	13.562460
H	1.246874	12.289010	12.637893
H	0.113326	11.584918	13.811744

C	-0.176790	7.149985	14.064229
C	-0.854688	5.757635	14.111044
H	-1.011214	5.499832	13.054707
C	0.137842	4.747107	14.707716
H	0.349166	4.984259	15.757385
H	1.088376	4.758344	14.164369
H	-0.277576	3.733776	14.668204
C	-2.207684	5.643118	14.811367
H	-2.657154	4.673413	14.569906
H	-2.896407	6.425142	14.470556
H	-2.115339	5.696843	15.901157
C	0.892407	7.225948	13.096920
H	0.771259	6.670118	12.172954
C	2.040191	7.944581	13.315168
H	2.801019	7.972451	12.539415
C	2.246978	8.626034	14.520658
H	3.158046	9.195598	14.667237
C	1.270821	8.606137	15.519036
C	1.459285	9.451955	16.769960
H	0.808190	9.063795	17.560135
C	1.023196	10.899821	16.500512
H	1.660452	11.357945	15.735928
H	1.098640	11.497722	17.416786
H	-0.010401	10.941277	16.138135
C	2.890940	9.402960	17.314519
H	3.598592	9.909683	16.650302
H	3.233684	8.371996	17.451223
H	2.935477	9.912811	18.282780
C	0.100123	7.873248	15.290242
C	-5.265922	7.277366	16.616261
H	-4.240896	6.896115	16.560767
C	-5.813872	7.324386	15.182943
H	-6.854095	7.668994	15.170126
H	-5.780848	6.327085	14.730109
H	-5.218551	8.005950	14.567471
C	-6.072126	6.307913	17.490064
H	-5.687409	6.281535	18.515058
H	-6.018381	5.295357	17.075920
H	-7.129132	6.591870	17.534847

Calculated energies and coordinates of **C**

Electronic energy ... -4000.69366596 Eh
Total Enthalpy ... -3999.46913916 Eh
Final Gibbs free energy ... -3999.64150517 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.197257	9.041171	9.546922
Si	-1.237618	10.283708	11.291145
Si	-1.392632	8.918484	13.206173
P	-2.691110	9.825262	14.720996
Si	-3.522186	10.607566	10.666333
Si	-0.323994	12.438385	11.702280
N	-2.860909	8.387651	17.127618
N	-0.857544	8.278954	16.257296
C	-3.083934	10.065627	4.124522
H	-3.968297	10.692628	4.292316
H	-3.420144	9.139612	3.649771
H	-2.436778	10.598466	3.420658
C	-2.372273	9.790641	5.420795
C	-2.547321	8.584903	6.100357
H	-3.186873	7.816921	5.670354
C	-1.906836	8.345755	7.313629
H	-2.047734	7.385452	7.805426
C	-1.074800	9.307098	7.896865
C	-2.124846	8.773864	16.033054
C	-4.229626	8.751512	17.342412
C	-4.493769	9.938263	18.041011
C	-3.387768	10.850310	18.537975
H	-2.424713	10.420028	18.240974
C	-3.398741	10.952343	20.069038
H	-4.322492	11.419699	20.427724
H	-2.557944	11.563202	20.415268
H	-3.320735	9.963849	20.534089
C	-6.853583	9.460883	17.782383
H	-7.888989	9.739466	17.957071
C	-6.560408	8.300825	17.077825
H	-7.370355	7.682017	16.701889
C	-5.239441	7.920155	16.839672
C	-5.831432	10.271654	18.256950
H	-6.075489	11.183195	18.795247
C	-3.481142	12.236711	17.886456
H	-3.468146	12.151261	16.795477
H	-2.630290	12.854705	18.193950
H	-4.399267	12.756177	18.182629
C	-2.063799	7.701537	18.023614
H	-2.460046	7.309832	18.947414
C	-0.824216	7.622074	17.482546
H	0.066325	7.123983	17.830953
C	-0.257428	7.203370	9.980346
C	-1.447487	6.595179	10.407421
H	-2.355385	7.185967	10.495224
C	-1.497322	5.242041	10.723805
H	-2.437465	4.800996	11.049068
C	-0.351535	4.446851	10.654095
C	0.839435	5.045930	10.237172
H	1.745638	4.446901	10.174876
C	0.884423	6.395592	9.901007
H	1.828645	6.830591	9.579632
C	-0.388780	3.000143	11.063133
H	0.357328	2.411905	10.520820
H	-1.374052	2.559898	10.883252
H	-0.172738	2.896098	12.134250
C	-1.525542	10.748446	5.988009
H	-1.363346	11.692130	5.470809
C	-0.893901	10.512563	7.201738
H	-0.240380	11.279592	7.614440
C	1.597285	9.542094	9.257805
C	2.213481	9.313962	8.019256
H	1.641075	8.873304	7.205391
C	3.547138	9.646686	7.807075
H	4.000519	9.455668	6.836590
C	4.314653	10.227662	8.819864
C	5.744579	10.626021	8.576830
H	5.807200	11.675011	8.261774

H	6.199081	10.018765	7.788728
H	6.346753	10.521122	9.484355
C	3.706262	10.455959	10.056256
H	4.282749	10.908527	10.861393
C	2.374451	10.117931	10.266924
H	1.924617	10.299927	11.238558
C	-4.606916	11.293255	12.052345
H	-4.193302	12.184730	12.530281
H	-4.779144	10.548021	12.834933
H	-5.579448	11.562473	11.619366
C	-4.357871	9.004611	10.113875
H	-5.400168	9.224359	9.849299
H	-4.373004	8.264316	10.922097
H	-3.878406	8.562545	9.235047
C	-3.591785	11.833346	9.229312
H	-3.089174	11.443112	8.339319
H	-3.128684	12.791797	9.488018
H	-4.640309	12.029020	8.970820
C	0.277258	13.240088	10.099482
H	-0.530736	13.314484	9.363162
H	1.093219	12.661846	9.652084
H	0.647994	14.253860	10.297047
C	-1.666698	13.530367	12.459698
H	-2.050127	13.092775	13.388492
H	-2.510361	13.686491	11.780468
H	-1.241667	14.513091	12.700229
C	1.083553	12.391767	12.960701
H	1.245831	13.402754	13.356107
H	2.029095	12.046638	12.532471
H	0.837986	11.732380	13.799793
C	0.145014	7.893944	14.025073
C	-0.067811	6.354913	13.929571
H	0.005555	6.136940	12.855200
C	1.077268	5.627917	14.641304
H	1.036438	5.801951	15.723416
H	2.049743	5.979586	14.281150
H	1.013710	4.546982	14.472584
C	-1.424392	5.837249	14.400069
H	-1.562074	4.801206	14.069209
H	-2.240155	6.434787	13.970668
H	-1.515570	5.849889	15.491964
C	1.272811	8.338390	13.174954
H	1.285524	7.968990	12.152540
C	2.320394	9.079832	13.647490
H	3.138278	9.317770	12.970985
C	2.365326	9.548646	14.968620
H	3.186773	10.178506	15.287348
C	1.295990	9.292552	15.832159
C	1.212364	10.032941	17.161270
H	0.617878	9.443249	17.866643
C	0.468538	11.362858	16.949397
H	1.047813	12.021094	16.292015
H	0.320049	11.876728	17.906927
H	-0.510294	11.204808	16.480893
C	2.572929	10.267467	17.822275
H	3.179832	10.987779	17.264138
H	3.144076	9.337274	17.909885
H	2.429201	10.678266	18.827380
C	0.248947	8.485904	15.387518
C	-4.934205	6.663512	16.049904
H	-3.847126	6.541103	16.010187
C	-5.431793	6.792717	14.603455
H	-6.524119	6.874327	14.565610
H	-5.139289	5.909893	14.023775
H	-5.001003	7.678888	14.126481
C	-5.516408	5.417275	16.729607
H	-5.156431	5.320878	17.759436
H	-5.225388	4.516732	16.178066
H	-6.611008	5.451995	16.758155

Calculated energies and coordinates of **TS[C-D]**

Electronic energy ... -4000.69037875 Eh
Total Enthalpy ... -3999.46667292 Eh
Final Gibbs free energy ... -3999.63700435 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.125339	9.110677	9.658202
Si	-0.972391	10.512964	11.394830
Si	-1.193056	9.152979	13.289116
P	-3.011686	9.403166	14.497760
Si	-3.243644	11.067330	10.872198
Si	0.204736	12.568671	11.617747
N	-2.937689	8.143101	17.008772
N	-0.938420	8.452555	16.156615
C	-3.293304	10.437410	4.465102
H	-4.032206	11.214889	4.695286
H	-3.835131	9.573045	4.070863
H	-2.645069	10.828294	3.674681
C	-2.503188	10.076843	5.692921
C	-2.832686	8.960288	6.462362
H	-3.653740	8.318615	6.149414
C	-2.120902	8.650152	7.617816
H	-2.390606	7.758898	8.180640
C	-1.058547	9.449825	8.052939
C	-2.281294	8.627940	15.900577
C	-4.344306	8.303864	17.224395
C	-4.789443	9.503797	17.800124
C	-3.837954	10.617958	18.194509
H	-2.822252	10.324350	17.908857
C	-3.845248	10.834747	19.714164
H	-4.828977	11.168668	20.062239
H	-3.112981	11.601053	19.990957
H	-3.595376	9.911702	20.248031
C	-7.047674	8.643886	17.640897
H	-8.113252	8.777213	17.805344
C	-6.579857	7.472656	17.060816
H	-7.285095	6.698723	16.771453
C	-5.216102	7.276390	16.838978
C	-6.161739	9.648198	18.006730
H	-6.541792	10.562574	18.453707
C	-4.159127	11.918833	17.447018
H	-4.142669	11.757195	16.364745
H	-3.414870	12.684714	17.691918
H	-5.144858	12.307268	17.726380

C	-2.017607	7.718831	17.952639
H	-2.330365	7.310960	18.901328
C	-0.783412	7.887850	17.423367
H	0.185592	7.608419	17.803914
C	-0.375142	7.301381	10.135600
C	-1.592031	6.849422	10.665827
H	-2.405115	7.551617	10.834030
C	-1.791715	5.509854	10.984075
H	-2.749502	5.193070	11.391400
C	-0.772121	4.573219	10.811179
C	0.447657	5.016911	10.292799
H	1.258041	4.304729	10.149966
C	0.641059	6.352920	9.957134
H	1.602732	6.663974	9.554113
C	-0.961358	3.135091	11.208579
H	-0.494468	2.457317	10.486886
H	-2.021682	2.878836	11.286587
H	-0.499604	2.938520	12.184515
C	-1.426141	10.866012	6.107946
H	-1.139805	11.733938	5.517209
C	-0.722338	10.561514	7.265783
H	0.109949	11.198270	7.559362
C	1.699137	9.392245	9.275228
C	2.222741	9.059506	8.017490
H	1.562391	8.675219	7.242644
C	3.575901	9.215739	7.737296
H	3.955491	8.946537	6.753738
C	4.457730	9.716369	8.698692
C	5.913199	9.922760	8.380484
H	6.086050	10.934232	7.992259
H	6.258939	9.216505	7.620051
H	6.536598	9.803506	9.271586
C	3.942180	10.048130	9.953478
H	4.608886	10.440435	10.719502
C	2.589639	9.887698	10.232145
H	2.212085	10.149141	11.216354
C	-4.062068	12.113772	12.218433
H	-3.711152	13.148836	12.197902
H	-3.898384	11.718661	13.225143
H	-5.144080	12.123023	12.033975
C	-4.314182	9.527742	10.638548
H	-5.345919	9.846315	10.441934
H	-4.327480	8.898268	11.535552
H	-3.987301	8.926025	9.784586
C	-3.315121	12.071849	9.274324
H	-3.003788	11.484348	8.406102
H	-2.683879	12.966136	9.322231
H	-4.348728	12.403847	9.111573
C	0.776132	13.153422	9.914413
H	-0.064266	13.227766	9.215401
H	1.514955	12.466355	9.487652
H	1.239013	14.145402	9.991767
C	-0.959355	13.875406	12.328321
H	-1.428097	13.540926	13.259903
H	-1.753776	14.133321	11.621248
H	-0.391359	14.789595	12.541631
C	1.689509	12.478260	12.780194
H	1.981569	13.498343	13.060936
H	2.557624	12.000839	12.316604
H	1.453847	11.923674	13.693899
C	0.180151	7.992561	13.965646
C	0.040691	6.449756	13.994335
H	0.196350	6.147607	12.948626
C	1.158947	5.832622	14.842155
H	1.038231	6.103495	15.897991
H	2.144979	6.178526	14.516621
H	1.135518	4.739000	14.775216
C	-1.321368	5.905024	14.421005
H	-1.402308	4.848024	14.140241
H	-2.139268	6.447685	13.935615
H	-1.454522	5.964335	15.506906
C	1.412253	8.379508	13.207408
H	1.520892	7.928183	12.223202
C	2.411243	9.127234	13.729702
H	3.308100	9.291903	13.135644
C	2.317899	9.742632	15.012766
H	3.114800	10.399899	15.337363
C	1.166876	9.613424	15.753238
C	0.923266	10.482441	16.981411
H	0.477289	9.871991	17.775597
C	-0.103026	11.576097	16.632645
H	0.311361	12.255645	15.878730
H	-0.349046	12.165011	17.524283
H	-1.028302	11.155613	16.224720
C	2.190295	11.108506	17.563888
H	2.623486	11.849607	16.883123
H	2.953729	10.354219	17.781466
H	1.947617	11.627080	18.497243
C	0.111597	8.790504	15.254078
C	-4.723641	6.002318	16.183244
H	-3.629550	6.023266	16.183004
C	-5.179010	5.934321	14.718578
H	-6.271680	5.884453	14.647091
H	-4.766049	5.041189	14.235786
H	-4.836103	6.817346	14.169453
C	-5.163614	4.756650	16.962866
H	-4.844225	4.809575	18.008986
H	-4.725709	3.858204	16.514778
H	-6.252461	4.636854	16.949477

Calculated energies and coordinates of **D**

Electronic energy ... -4000.69880301 Eh
Total Enthalpy ... -3999.47389881 Eh
Final Gibbs free energy ... -3999.64478117 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	-0.129304	9.155241	9.740220
Si	-0.803528	10.600407	11.523491
Si	-1.059134	9.220999	13.411420
P	-3.112146	9.023470	14.259090
Si	-3.032092	11.350293	11.075659
Si	0.506748	12.586666	11.647634
N	-2.958488	8.048825	16.915257
N	-1.009378	8.521048	16.041874

C	-3.393588	10.621220	4.639736
H	-4.108090	11.415785	4.888134
H	-3.964773	9.773269	4.251395
H	-2.750913	11.000189	3.838974
C	-2.588739	10.232972	5.849580
C	-2.935024	9.124320	6.623059
H	-3.782860	8.509939	6.327341
C	-2.206255	8.786761	7.760283
H	-2.490635	7.901887	8.325889
C	-1.108867	9.550421	8.173748
C	-2.358512	8.529622	15.777704
C	-4.373451	8.084563	17.138752
C	-4.936709	9.283878	17.602178
C	-4.103368	10.522380	17.873335
H	-3.060652	10.300360	17.622357
C	-4.148251	10.902645	19.359732
H	-5.162937	11.176021	19.669717
H	-3.496550	11.762345	19.550391
H	-3.816087	10.072251	19.991887
C	-7.096318	8.188309	17.562687
H	-8.169210	8.229031	17.728761
C	-6.513501	7.017884	17.096785
H	-7.136685	6.150741	16.897102
C	-5.137851	6.939853	16.873770
C	-6.315667	9.308871	17.812934
H	-6.784801	10.220428	18.172532
C	-4.543397	11.693211	16.984615
H	-4.503622	11.410286	15.928177
H	-3.879277	12.551361	17.136585
H	-5.564654	12.012438	17.221071
C	-1.992751	7.763693	17.873658
H	-2.260379	7.382760	18.846988
C	-0.784742	8.036813	17.326311
H	0.209627	7.904628	17.721911
C	-0.473256	7.365268	10.227281
C	-1.698303	6.989626	10.794001
H	-2.460624	7.740503	10.991652
C	-1.969433	5.665267	11.122362
H	-2.929619	5.409471	11.565221
C	-1.017389	4.666917	10.915253
C	0.210908	5.034282	10.357273
H	0.970825	4.273040	10.190348
C	0.476957	6.356081	10.016931
H	1.442914	6.609048	9.584517
C	-1.286942	3.238326	11.301723
H	-1.145746	2.563705	10.449903
H	-2.308287	3.112061	11.671051
H	-0.599630	2.910543	12.090811
C	-1.477648	10.985819	6.241689
H	-1.177045	11.845985	5.646642
C	-0.756592	10.653579	7.381248
H	0.104532	11.260035	7.653803
C	1.691683	9.319350	9.275784
C	2.131149	8.998384	7.983064
H	1.409445	8.692698	7.228375
C	3.478009	9.065952	7.643160
H	3.790620	8.808351	6.633211
C	4.438453	9.461703	8.577904
C	5.888982	9.573356	8.195892
H	6.111166	10.573511	7.803496
H	6.152763	8.850892	7.417810
H	6.541978	9.406914	9.057667
C	4.007426	9.778264	9.867984
H	4.736349	10.086900	10.615354
C	2.660608	9.707630	10.206017
H	2.351287	9.951253	11.218157
C	-3.732573	12.325821	12.534942
H	-3.266994	13.309431	12.638661
H	-3.608154	11.781390	13.476472
H	-4.807789	12.476619	12.373428
C	-4.212934	9.919436	10.722499
H	-5.211306	10.331870	10.527219
H	-4.301153	9.230755	11.569442
H	-3.908442	9.356608	9.834505
C	-3.048772	12.473240	9.555898
H	-2.766475	11.927468	8.650243
H	-2.375510	13.330486	9.660296
H	-4.064592	12.864568	9.414963
C	0.983536	13.083527	9.888352
H	0.102600	13.183304	9.245280
H	1.655811	12.345781	9.436832
H	1.501609	14.050787	9.903710
C	-0.521111	13.987045	12.393966
H	-0.926043	13.719305	13.375528
H	-1.358355	14.271049	11.749425
H	0.117429	14.870324	12.521643
C	2.073173	12.490463	12.693864
H	2.529671	13.488363	12.724189
H	2.815666	11.793810	12.296030
H	1.844213	12.185172	13.719161
C	0.259224	7.939014	13.924058
C	0.136883	6.408647	14.079378
H	0.335823	6.033459	13.063908
C	1.234769	5.867577	15.007249
H	1.072580	6.211764	16.035539
H	2.229452	6.199020	14.693663
H	1.222782	4.771418	15.019756
C	-1.219837	5.843451	14.497645
H	-1.244918	4.767880	14.284132
H	-2.044563	6.318484	13.961400
H	-1.384874	5.962120	15.573952
C	1.546477	8.267550	13.269877
H	1.780469	7.687461	12.377675
C	2.450107	9.135856	13.763859
H	3.395647	9.273803	13.244314
C	2.218605	9.888334	14.975927
H	2.997977	10.562301	15.313814
C	1.033656	9.831449	15.623621
C	0.672134	10.775184	16.756547
H	0.250388	10.198480	17.590834
C	-0.432400	11.739731	16.282528
H	-0.055353	12.366932	15.465879
H	-0.741273	12.396571	17.103843
H	-1.315289	11.209161	15.911081
C	1.857937	11.562606	17.312112
H	2.264320	12.255240	16.566036

H	2.665821	10.901698	17.643263
H	1.533985	12.159803	18.170610
C	-0.034957	8.970608	15.071342
C	-4.521739	5.662485	16.341009
H	-3.435988	5.793647	16.323933
C	-4.973601	5.400806	14.896984
H	-6.054068	5.221838	14.849209
H	-4.464547	4.516199	14.497325
H	-4.736151	6.257362	14.257852
C	-4.829364	4.462696	17.246102
H	-4.513426	4.651158	18.277586
H	-4.303453	3.573204	16.882681
H	-5.900216	4.232123	17.259312

Calculated energies and coordinates of **TS[D-E]**

Electronic energy ... -4000.67943915 Eh
Total Enthalpy ... -3999.45618353 Eh
Final Gibbs free energy ... -3999.62551697 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	1.335952	0.004819	-3.252009
Si	0.086531	1.036736	-1.496693
Si	-0.134908	-0.276170	0.459576
P	-2.115206	-0.058546	1.485516
Si	-2.192027	1.285207	-2.212712
Si	0.699242	3.219401	-0.785077
N	-1.768312	-0.473399	4.261882
N	0.114484	-0.444594	3.143202
C	-1.465573	1.401760	-8.634627
H	-1.740479	0.509684	-9.204493
H	-0.837240	2.035808	-9.267870
H	-2.387318	1.959325	-8.426806
C	-0.764151	1.040767	-7.354042
C	-0.924050	-0.217944	-6.772772
H	-1.541026	-0.962320	-7.271826
C	-0.300745	-0.536478	-5.568873
H	-0.433639	-1.531888	-5.150066
C	0.501177	0.394488	-4.899598
C	-1.252942	-0.313064	3.001692
C	-3.147367	-0.287588	4.594227
C	-3.605791	1.017920	4.826501
C	-2.699734	2.229374	4.714280
H	-1.709126	1.891419	4.391273
C	-2.535106	2.920088	6.075251
H	-3.490996	3.314163	6.437895
H	-1.835748	3.759157	5.992685
H	-2.150823	2.224682	6.829051
C	-5.791347	0.077829	5.281408
H	-6.832405	0.221347	5.556932
C	-5.314471	-1.200949	5.027452
H	-5.988808	-2.049568	5.100432
C	-3.982121	-1.410822	4.669017
C	-4.947541	1.175428	5.175545
H	-5.336931	2.171715	5.365555
C	-3.211920	3.209116	3.650008
H	-3.320956	2.705026	2.684726
H	-2.502654	4.035014	3.527151
H	-4.180837	3.636136	3.932207
C	-0.741238	-0.721045	5.166912
H	-0.940473	-0.883083	6.214764
C	0.420260	-0.724883	4.474895
H	1.423074	-0.932578	4.806240
C	1.327442	-1.868239	-3.032483
C	0.185863	-2.553349	-2.597440
H	-0.717128	-1.998000	-2.350892
C	0.186073	-3.934228	-2.441270
H	-0.713593	-4.436896	-2.091625
C	1.334510	-4.685457	-2.704029
C	2.477221	-4.008767	-3.136270
H	3.386663	-4.571097	-3.338382
C	2.472677	-2.627105	-3.302265
H	3.384094	-2.129074	-3.625967
C	1.330668	-6.180817	-2.540601
H	0.964449	-6.671318	-3.451000
H	0.676808	-6.488797	-1.718710
H	2.336484	-6.562867	-2.343077
C	0.050282	1.969685	-6.698654
H	0.197871	2.954302	-7.137952
C	0.665612	1.653641	-5.495092
H	1.296763	2.398515	-5.012687
C	3.120547	0.587199	-3.433634
C	3.746370	0.549511	-4.689181
H	3.179590	0.242046	-5.565457
C	5.084221	0.898264	-4.838788
H	5.543590	0.854739	-5.824258
C	5.848579	1.305815	-3.742468
C	7.284264	1.721610	-3.911763
H	7.752412	1.204147	-4.754338
H	7.868270	1.513086	-3.010413
H	7.356177	2.798854	-4.107155
C	5.231746	1.343543	-2.490362
H	5.804289	1.657438	-1.619364
C	3.895184	0.990439	-2.342001
H	3.446249	1.019868	-1.354815
C	-3.168069	2.398747	-1.035883
H	-2.821204	3.436174	-1.085942
H	-3.119653	2.066584	0.004795
H	-4.220234	2.387381	-1.348978
C	-3.056824	-0.394114	-2.303747
H	-4.123476	-0.242663	-2.511973
H	-2.978673	-0.956295	-1.366302
H	-2.646598	-1.005508	-3.115477
C	-2.344641	2.092316	-3.912947
H	-2.058371	1.414586	-4.720889
H	-1.737527	2.997675	-4.006022
H	-3.395352	2.376040	-4.058086
C	0.093397	4.497369	-2.041067
H	-0.994120	4.486120	-2.158751
H	0.539216	4.323866	-3.026939
H	0.386509	5.503350	-1.715101
C	-0.148717	3.524422	0.877009
H	0.118274	2.752560	1.607777
H	-1.238610	3.511725	0.785961
H	0.152701	4.500640	1.278544

C	2.548805	3.519985	-0.569758
H	2.693779	4.503111	-0.102805
H	3.071136	3.518674	-1.531400
H	3.015717	2.768566	0.072931
C	0.833393	-1.868626	0.735086
C	0.285598	-3.242073	1.144200
H	0.777476	-3.927796	0.435632
C	0.754736	-3.655049	2.546509
H	0.221786	-3.094864	3.321759
H	1.828217	-3.474916	2.668323
H	0.559711	-4.720469	2.715736
C	-1.217781	-3.453049	0.984986
H	-1.455825	-4.518129	1.096150
H	-1.563285	-3.125681	-0.001394
H	-1.790677	-2.892586	1.726668
C	2.132626	-1.928230	0.137285
H	2.332057	-2.839271	-0.428569
C	3.154141	-1.023615	0.225054
H	4.036645	-1.206851	-0.383067
C	3.243003	-0.008761	1.211784
H	4.199987	0.500787	1.303819
C	2.289895	0.224626	2.168698
C	2.659612	1.075476	3.386255
H	1.765874	1.209913	4.005073
C	3.111568	2.485920	2.981347
H	4.027808	2.459316	2.382224
H	3.319409	3.083090	3.876933
H	2.341768	2.997724	2.398345
C	3.749208	0.411262	4.242707
H	4.695990	0.379550	3.692935
H	3.501606	-0.623752	4.500988
H	3.914706	0.971597	5.170542
C	0.959417	-0.303557	2.002627
C	-3.481987	-2.809201	4.367618
H	-2.440409	-2.733675	4.036019
C	-4.281967	-3.448222	3.224883
H	-5.325244	-3.617300	3.513581
H	-3.847302	-4.417300	2.956982
H	-4.269626	-2.807520	2.337510
C	-3.507184	-3.689512	5.624618
H	-2.916428	-3.245109	6.432648
H	-3.096175	-4.680584	5.403717
H	-4.530765	-3.823053	5.992429

Calculated energies and coordinates of **E**

Electronic energy ... -4000.70639384 Eh
Total Enthalpy ... -3999.48138666 Eh
Final Gibbs free energy ... -3999.65187977 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	1.351564	0.010957	-3.135504
Si	-0.050286	0.673113	-1.305419
Si	-0.090377	-0.747888	0.631417
P	-2.059303	-0.556104	1.698473
Si	-2.319637	0.811991	-2.094091
Si	0.286263	2.883567	-0.476876
N	-1.650544	0.269012	4.338714
N	0.241917	0.098641	3.213386
C	-1.172056	2.009865	-8.467454
H	-1.297607	1.206168	-9.198535
H	-0.571548	2.802068	-8.925325
H	-2.164773	2.429572	-8.262596
C	-0.537522	1.505301	-7.200577
C	-0.598715	0.156418	-6.848966
H	-1.085494	-0.548853	-7.519458
C	-0.041786	-0.300944	-5.657231
H	-0.095937	-1.361377	-5.421043
C	0.593754	0.575295	-4.771055
C	-1.146517	-0.035769	3.099945
C	-3.041401	0.245580	4.673260
C	-3.781074	1.428985	4.539372
C	-3.158505	2.709136	4.019536
H	-2.175529	2.466639	3.601585
C	-2.948386	3.712761	5.162515
H	-3.906825	4.003853	5.607670
H	-2.456800	4.618062	4.789619
H	-2.325414	3.286789	5.956199
C	-5.699059	0.227667	5.399802
H	-6.745002	0.222132	5.693517
C	-4.949739	-0.937139	5.493884
H	-5.418173	-1.847893	5.856066
C	-3.603721	-0.955889	5.126145
C	-5.122291	1.396858	4.922221
H	-5.723330	2.297778	4.840672
C	-3.988465	3.328095	2.888857
H	-4.164245	2.601510	2.089658
H	-3.456402	4.184392	2.461155
H	-4.959483	3.686818	3.247353
C	-0.616285	0.539757	5.220272
H	-0.804763	0.780478	6.255025
C	0.547000	0.428884	4.545915
H	1.545559	0.537986	4.921058
C	1.493897	-1.870071	-3.193420
C	0.358143	-2.682113	-3.084525
H	-0.617629	-2.221040	-2.944466
C	0.448068	-4.067268	-3.123371
H	-0.453361	-4.670049	-3.030436
C	1.686674	-4.700315	-3.255984
C	2.824516	-3.898965	-3.360417
H	3.801112	-4.368663	-3.460138
C	2.729456	-2.509995	-3.337354
H	3.636769	-1.915340	-3.419252
C	1.781477	-6.200847	-3.302352
H	1.539456	-6.576548	-4.304219
H	1.078311	-6.664815	-2.603183
H	2.789913	-6.544977	-3.055687
C	0.116366	2.382457	-6.329657
H	0.191136	3.436644	-6.589396
C	0.668166	1.925880	-5.140870
H	1.182077	2.633285	-4.491708
C	3.098703	0.727746	-3.151259
C	3.812184	0.767706	-4.359433
H	3.330953	0.444279	-5.280396
C	5.127661	1.214948	-4.405661

H	5.656731	1.229781	-5.356436
C	5.781900	1.649696	-3.249496
C	7.192119	2.169862	-3.308713
H	7.760691	1.689584	-4.110621
H	7.718791	2.003306	-2.364340
H	7.200062	3.249659	-3.502790
C	5.076222	1.616630	-2.045658
H	5.559915	1.953687	-1.130037
C	3.761784	1.163851	-2.002728
H	3.237807	1.143132	-1.054705
C	-3.415049	1.778559	-0.892593
H	-3.092446	2.816376	-0.764985
H	-3.449228	1.304025	0.092513
H	-4.433133	1.795247	-1.303360
C	-3.122741	-0.887780	-2.293769
H	-4.183861	-0.751636	-2.538254
H	-3.066677	-1.478644	-1.374593
H	-2.671845	-1.465958	-3.107347
C	-2.473126	1.695592	-3.756593
H	-2.096362	1.091171	-4.585690
H	-1.945161	2.652920	-3.779980
H	-3.538689	1.893696	-3.932697
C	-0.390439	4.163093	-1.695495
H	-1.468692	4.066944	-1.851325
H	0.096130	4.082828	-2.673609
H	-0.195258	5.170898	-1.307301
C	-0.623454	3.054419	1.172110
H	-0.063683	2.539079	1.961225
H	-1.630764	2.631968	1.152068
H	-0.690960	4.115678	1.445610
C	2.068382	3.385721	-0.110808
H	2.054584	4.352430	0.409335
H	2.679113	3.489889	-1.012109
H	2.547613	2.656442	0.549815
C	0.520341	-2.511750	0.367042
C	-0.304905	-3.772021	0.544859
H	0.262866	-4.586460	0.067221
C	-0.428738	-4.103930	2.042253
H	-0.974816	-3.305081	2.556617
H	0.558911	-4.201507	2.504216
H	-0.978740	-5.042447	2.182998
C	-1.690131	-3.724036	-0.102588
H	-2.174961	-4.704513	-0.030724
H	-1.626701	-3.453599	-1.159621
H	-2.335584	-2.999797	0.405911
C	1.836170	-2.635813	0.066370
H	2.188375	-3.628583	-0.234474
C	2.863375	-1.634003	0.026053
H	3.662815	-1.848762	-0.682958
C	3.098751	-0.555694	0.832415
H	4.059098	-0.082336	0.647646
C	2.386689	-0.041906	1.973928
C	3.263421	0.574162	3.065332
H	2.658035	1.312767	3.601718
C	4.487651	1.350090	2.557966
H	5.261614	0.687869	2.157440
H	4.933470	1.896818	3.395850
H	4.223668	2.080707	1.787200
C	3.731309	-0.524402	4.036628
H	4.404852	-1.209530	3.510044
H	2.898911	-1.124289	4.417654
H	4.276548	-0.097559	4.887343
C	1.025175	-0.173280	2.070070
C	-2.799031	-2.236652	5.230648
H	-1.807881	-2.054418	4.800710
C	-3.443394	-3.368641	4.420458
H	-4.423201	-3.644763	4.825224
H	-2.806837	-4.259635	4.448417
H	-3.569592	-3.069114	3.375264
C	-2.607512	-2.642391	6.698771
H	-2.127529	-1.842256	7.272226
H	-1.981771	-3.538820	6.768563
H	-3.569755	-2.864591	7.173840

Calculated energies and coordinates of **TS[A-F]**

Electronic energy ... -4057.21572926 Eh
Total Enthalpy ... -4055.95635514 Eh
Final Gibbs free energy ... -4056.13297456 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.654597	-0.172440	-3.603206
Si	-0.590891	0.880913	-1.879717
Si	0.508676	0.107739	0.058516
P	-0.798109	0.772468	1.753631
Si	-2.814765	0.072201	-1.807151
Si	-0.623636	3.245317	-2.030262
N	-1.232662	-0.401833	4.210328
N	0.760446	-0.951167	3.534288
N	2.208003	0.971510	-0.073080
C	-0.024203	2.616876	-9.128704
H	-1.065213	2.599344	-9.464902
H	0.595227	2.147255	-9.898437
H	0.279707	3.668783	-9.058598
C	0.134168	1.926921	-7.801342
C	1.322419	1.271828	-7.468733
H	2.133424	1.237360	-8.193451
C	1.482522	0.663951	-6.228058
H	2.421200	0.163027	-5.999909
C	0.459810	0.687743	-5.269688
C	-0.360578	-0.245271	3.146933
C	-2.511970	0.240003	4.322574
C	-2.583672	1.460324	5.005771
C	-1.356934	2.155779	5.565182
H	-0.501100	1.480106	5.460552
C	-1.509061	2.465538	7.059883
H	-2.302797	3.198305	7.240720
H	-0.577054	2.885262	7.453820
H	-1.748843	1.563031	7.632031
C	-4.968743	1.453606	4.595707
H	-5.938310	1.932611	4.699134
C	-4.866294	0.244474	3.916901
H	-5.758268	-0.203217	3.492044
C	-3.635403	-0.390175	3.763375
C	-3.841171	2.054861	5.132220

H	-3.933463	3.005329	5.649852
C	-1.039516	3.425556	4.762266
H	-0.883429	3.185295	3.705152
H	-0.132061	3.901219	5.152058
H	-1.858268	4.150428	4.834461
C	-0.644016	-1.134226	5.229048
H	-1.163836	-1.338447	6.151825
C	0.591701	-1.479178	4.810122
H	1.371406	-2.049877	5.288972
C	0.116398	-1.973948	-3.765322
C	-0.297437	-2.502206	-4.994386
H	-0.317093	-1.862459	-5.874340
C	-0.692747	-3.831718	-5.112722
H	-1.016819	-4.211682	-6.079481
C	-0.680437	-4.686266	-4.009472
C	-0.274039	-4.163837	-2.778383
H	-0.277173	-4.804412	-1.898063
C	0.110128	-2.834209	-2.655653
H	0.383159	-2.447197	-1.672739
C	-1.074688	-6.132183	-4.141522
H	-1.591521	-6.487164	-3.244495
H	-0.190266	-6.766246	-4.281835
H	-1.731472	-6.289117	-5.002021
C	-0.892945	1.946673	-6.855001
H	-1.831098	2.444646	-7.092360
C	-0.729457	1.341082	-5.614315
H	-1.545698	1.373854	-4.897014
C	2.490800	-0.127466	-3.152395
C	3.217636	1.065093	-3.291754
H	2.756126	1.921198	-3.778113
C	4.517362	1.184031	-2.814944
H	5.051510	2.125034	-2.935317
C	5.151546	0.107402	-2.185235
C	6.541290	0.254040	-1.628548
H	6.979588	-0.719146	-1.388904
H	6.531565	0.853001	-0.708961
H	7.204221	0.761823	-2.336897
C	4.452892	-1.094072	-2.084323
H	4.935294	-1.954099	-1.624151
C	3.146962	-1.210483	-2.555108
H	2.635708	-2.164424	-2.456980
C	-3.846457	1.139543	-0.636737
H	-3.859884	2.191099	-0.942292
H	-3.448953	1.090891	0.383649
H	-4.884977	0.783552	-0.624874
C	-2.874543	-1.714217	-1.205756
H	-3.918696	-2.030826	-1.090225
H	-2.373766	-1.823239	-0.236907
H	-2.390553	-2.386203	-1.920795
C	-3.628741	0.111879	-3.515917
H	-3.073382	-0.500697	-4.235327
H	-3.704431	1.128850	-3.916264
H	-4.646197	-0.293716	-3.447054
C	-2.047915	3.881442	-3.104720
H	-3.017476	3.481716	-2.791102
H	-1.897539	3.623442	-4.158289
H	-2.099379	4.975539	-3.034037
C	-0.832396	3.949712	-0.290914
H	0.006922	3.663744	0.352958
H	-1.743389	3.576249	0.189012
H	-0.885552	5.045346	-0.325898
C	0.964273	3.952834	-2.776015
H	0.906255	5.048528	-2.797488
H	1.100165	3.603944	-3.806041
H	1.852553	3.675712	-2.198183
C	2.430173	-2.038339	2.102148
C	1.622032	-3.304274	1.840910
H	1.921024	-3.613044	0.829000
C	2.077902	-4.408536	2.812017
H	1.799271	-4.153155	3.840890
H	3.162300	-4.554110	2.780381
H	1.591752	-5.357810	2.561128
C	0.093380	-3.210275	1.831021
H	-0.308985	-4.110294	1.352461
H	-0.248797	-2.340223	1.262168
H	-0.326334	-3.163856	2.841334
C	3.717481	-1.996762	1.555310
H	4.039431	-2.819157	0.921138
C	4.576056	-0.935540	1.791916
H	5.566674	-0.931093	1.345802
C	4.165018	0.128869	2.584715
H	2.820856	1.015066	0.731623
H	4.843765	0.956177	2.772716
C	2.886165	0.147190	3.145444
C	2.463264	1.316620	4.015743
H	1.406916	1.192422	4.270081
C	2.582514	2.654290	3.275331
H	3.618878	2.871438	2.992432
H	2.237056	3.468935	3.920560
H	1.963090	2.652901	2.372526
C	3.261669	1.328608	5.326767
H	4.329391	1.489062	5.139213
H	3.152790	0.380145	5.863377
H	2.908652	2.135023	5.979101
C	2.039196	-0.945688	2.888956
C	-3.507596	-1.716313	3.038383
H	-2.537677	-1.710485	2.524521
C	-4.584495	-1.922392	1.971855
H	-5.574040	-2.077211	2.416960
H	-4.349223	-2.813531	1.381915
H	-4.635277	-1.069681	1.288623
C	-3.525533	-2.889140	4.032228
H	-2.717747	-2.819337	4.766751
H	-3.411404	-3.838753	3.497513
H	-4.477527	-2.914770	4.575451
H	2.014067	-0.401005	-0.282435
H	2.519589	1.558219	-0.840140

Calculated energies and coordinates of **F**

Electronic energy ... -4057.31523585 Eh
Total Enthalpy ... -4056.05221421 Eh
Final Gibbs free energy ... -4056.22845968 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.676335	-0.150949	-3.612539
Si	-0.606234	0.832928	-1.877073
Si	0.594693	0.258963	0.072967
P	-0.819296	0.714875	1.752488
Si	-2.799659	-0.051118	-1.780210
Si	-0.675484	3.197271	-2.003205
N	-1.225992	-0.338654	4.252760
N	0.762557	-0.926776	3.588497
N	2.048794	1.229601	0.045202
C	0.025146	2.788855	-9.061779
H	-1.003305	2.725066	-9.429623
H	0.691488	2.378173	-9.826055
H	0.268083	3.853000	-8.951020
C	0.183582	2.067282	-7.751393
C	1.396873	1.470154	-7.401277
H	2.229662	1.503659	-8.100912
C	1.554491	0.832318	-6.175052
H	2.511975	0.374392	-5.935496
C	0.504417	0.769196	-5.248901
C	-0.356413	-0.228632	3.179032
C	-2.507036	0.303119	4.333970
C	-2.578768	1.578067	4.908932
C	-1.349362	2.332703	5.375209
H	-0.471642	1.705178	5.188850
C	-1.403958	2.614032	6.882694
H	-2.240371	3.275537	7.133790
H	-0.480713	3.103838	7.211265
H	-1.525157	1.688611	7.455956
C	-4.974313	1.506802	4.571161
H	-5.948164	1.978958	4.665934
C	-4.870665	0.252358	3.980518
H	-5.765669	-0.236884	3.610959
C	-3.634233	-0.375842	3.843722
C	-3.841345	2.164124	5.024313
H	-3.933308	3.152534	5.465779
C	-1.161899	3.626296	4.570560
H	-1.095248	3.406764	3.500174
H	-0.240549	4.132321	4.880026
H	-1.994993	4.319280	4.732813
C	-0.632424	-1.028356	5.299000
H	-1.147363	-1.190706	6.232731
C	0.599339	-1.397051	4.888681
H	1.379166	-1.949485	5.388395
C	0.147937	-1.944067	-3.880462
C	-0.191160	-2.418645	-5.154045
H	-0.160079	-1.741355	-6.004856
C	-0.576809	-3.741012	-5.353461
H	-0.842082	-4.077680	-6.353608
C	-0.630230	-4.643535	-4.290137
C	-0.298551	-4.176378	-3.015556
H	-0.351154	-4.855228	-2.166164
C	0.076462	-2.853375	-2.814266
H	0.295490	-2.517173	-1.801652
C	-1.013756	-6.081619	-4.509623
H	-1.556884	-6.484601	-3.649263
H	-0.122275	-6.704435	-4.655148
H	-1.642234	-6.195251	-5.397651
C	-0.871257	1.997732	-6.838178
H	-1.829340	2.447843	-7.090822
C	-0.710333	1.363803	-5.611555
H	-1.550026	1.326055	-4.921466
C	2.503399	-0.126519	-3.117109
C	3.251309	1.057761	-3.225558
H	2.802075	1.938343	-3.677795
C	4.557811	1.136593	-2.759613
H	5.106409	2.071882	-2.854208
C	5.176563	0.031504	-2.165755
C	6.579145	0.133360	-1.631607
H	6.970979	-0.848165	-1.349569
H	6.613445	0.778687	-0.745035
H	7.256771	0.569725	-2.373272
C	4.449962	-1.155243	-2.079016
H	4.916615	-2.035240	-1.640935
C	3.139783	-1.233563	-2.543717
H	2.608615	-2.178363	-2.460319
C	-3.888703	1.043634	-0.689902
H	-3.942784	2.073391	-1.058323
H	-3.503597	1.070957	0.335901
H	-4.911011	0.643997	-0.665515
C	-2.822435	-1.794608	-1.059381
H	-3.860035	-2.135878	-0.954896
H	-2.357506	-1.807983	-0.066899
H	-2.294529	-2.502924	-1.704467
C	-3.563933	-0.129938	-3.509492
H	-2.951710	-0.735578	-4.187814
H	-3.682403	0.866134	-3.950667
H	-4.559336	-0.588745	-3.455973
C	-2.069708	3.806493	-3.131611
H	-3.037348	3.360136	-2.880482
H	-1.855093	3.587114	-4.182590
H	-2.169532	4.894901	-3.032533
C	-0.963981	3.882746	-0.269159
H	-0.136635	3.605761	0.393517
H	-1.885668	3.494777	0.177399
H	-1.032106	4.977681	-0.302999
C	0.937900	3.912289	-2.673169
H	0.890701	5.008606	-2.667064
H	1.111598	3.589188	-3.705976
H	1.789497	3.604273	-2.057477
C	2.367725	-2.053797	2.116358
C	1.543256	-3.320864	1.916553
H	1.790115	-3.653200	0.897896
C	2.049635	-4.403848	2.887181
H	1.833415	-4.117830	3.923094
H	3.129509	-4.556819	2.796006
H	1.544593	-5.356110	2.690723
C	0.014773	-3.232464	1.990673
H	-0.407946	-4.145341	1.556003
H	-0.377481	-2.379350	1.431394
H	-0.344044	-3.168950	3.023064
C	3.622462	-2.022039	1.499923
H	3.902972	-2.845091	0.847092
C	4.506720	-0.974180	1.701860
H	5.471194	-0.976403	1.201871
C	4.159803	0.078494	2.538500
H	2.688223	1.086754	0.817325

H	4.861818	0.891357	2.703209
C	2.910311	0.113280	3.158666
C	2.555582	1.271948	4.072661
H	1.545998	1.106941	4.460037
C	2.536636	2.609257	3.320788
H	3.518736	2.842962	2.893456
H	2.271648	3.418873	4.009664
H	1.801862	2.592446	2.510011
C	3.506089	1.322430	5.277376
H	4.533475	1.541375	4.966165
H	3.513972	0.369699	5.817617
H	3.192357	2.109240	5.971974
C	2.025954	-0.955285	2.917761
C	-3.504884	-1.743710	3.201520
H	-2.533035	-1.768879	2.692922
C	-4.576126	-2.009436	2.141740
H	-5.567438	-2.145265	2.588951
H	-4.334497	-2.928600	1.598733
H	-4.627607	-1.191825	1.416525
C	-3.525143	-2.854531	4.263416
H	-2.713431	-2.739885	4.987870
H	-3.415896	-3.835835	3.788018
H	-4.474943	-2.842865	4.810780
H	0.869909	-1.213509	-0.030140
H	2.579352	1.170168	-0.818291

Calculated energies and coordinates of **G**

Electronic energy ... -4113.82690866 Eh
Total Enthalpy ... -4112.51939254 Eh
Final Gibbs free energy ... -4112.70231004 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.680377	-0.128171	-3.636662
Si	-0.370555	0.569911	-1.621291
Si	0.596399	-0.591591	0.262965
P	-0.641505	0.632138	1.735473
Si	-2.587490	-0.297199	-1.640837
Si	-0.592614	2.937316	-1.737700
N	-1.550516	-0.053654	4.261158
N	0.444623	-0.877014	3.987348
N	2.385263	0.361931	0.313279
C	-0.843233	3.793817	-8.241055
H	-1.431009	3.312842	-9.029149
H	0.034897	4.257141	-8.700102
H	-1.459032	4.597874	-7.819194
C	-0.449521	2.809656	-7.173751
C	0.784334	2.897805	-6.528034
H	1.489147	3.671829	-6.825160
C	1.130014	2.006383	-5.516624
H	2.109734	2.095173	-5.052198
C	0.253502	0.996104	-5.099434
C	-0.543326	-0.177531	3.316264
C	-2.789055	0.642584	4.055504
C	-2.863783	1.991233	4.423207
C	-1.668089	2.755633	4.956098
H	-0.801799	2.086121	4.940411
C	-1.891738	3.194341	6.409569
H	-2.733031	3.892109	6.486421
H	-1.000225	3.699786	6.797359
H	-2.108949	2.336737	7.055380
C	-5.189671	1.963616	3.757275
H	-6.136476	2.482650	3.637216
C	-5.082804	0.628727	3.382845
H	-5.947225	0.124141	2.964814
C	-3.880729	-0.062618	3.521881
C	-4.092186	2.637655	4.268876
H	-4.183713	3.684937	4.543127
C	-1.330765	3.950984	4.056096
H	-1.174179	3.618611	3.025588
H	-0.416948	4.442995	4.408504
H	-2.133793	4.696364	4.061600
C	-1.157521	-0.587982	5.478487
H	-1.799779	-0.557011	6.344601
C	0.078483	-1.104918	5.310390
H	0.733113	-1.615778	5.998677
C	0.232771	-1.911830	-4.068205
C	-0.002480	-2.343008	-5.379862
H	0.028200	-1.625529	-6.197017
C	-0.268224	-3.680030	-5.663877
H	-0.448533	-3.985190	-6.692799
C	-0.303412	-4.637668	-4.648887
C	-0.053691	-4.216836	-3.339657
H	-0.070589	-4.945278	-2.530833
C	0.205859	-2.881558	-3.054864
H	0.388211	-2.583915	-2.021031
C	-0.627973	-6.075904	-4.948665
H	-1.696774	-6.272734	-4.798239
H	-0.076238	-6.754177	-4.290347
H	-0.389399	-6.331229	-5.985292
C	-1.319787	1.788195	-6.783485
H	-2.282902	1.686817	-7.280162
C	-0.977343	0.905619	-5.766563
H	-1.685882	0.131189	-5.488256
C	2.575629	-0.091420	-3.514856
C	3.260249	0.934604	-2.852932
H	2.692231	1.720020	-2.359219
C	4.650250	0.985513	-2.818207
H	5.148053	1.797605	-2.291512
C	5.417536	0.004948	-3.449579
C	6.920651	0.065423	-3.437984
H	7.290180	0.641544	-2.584777
H	7.297393	0.546359	-4.349171
H	7.359620	-0.936132	-3.394019
C	4.745465	-1.021850	-4.118805
H	5.320916	-1.798092	-4.620296
C	3.354489	-1.067858	-4.152950
H	2.863582	-1.885091	-4.677711
C	-3.747459	0.825752	-0.654544
H	-3.809905	1.828880	-1.089900
H	-3.409200	0.923919	0.383315
H	-4.760636	0.402439	-0.655986
C	-2.629934	-2.020779	-0.865083
H	-3.659969	-2.399252	-0.863453
H	-2.267319	-1.998416	0.168352

H	-2.012030	-2.724603	-1.431273
C	-3.331088	-0.476946	-3.371985
H	-2.765127	-1.199591	-3.970818
H	-3.361557	0.476296	-3.909789
H	-4.360432	-0.847942	-3.284592
C	-1.762260	3.434545	-3.139671
H	-2.746237	2.964607	-3.038278
H	-1.355029	3.149937	-4.115394
H	-1.907247	4.522710	-3.132836
C	-1.239616	3.673084	-0.121562
H	-0.507349	3.535030	0.680961
H	-2.170774	3.208702	0.214644
H	-1.412189	4.749319	-0.254486
C	1.045909	3.838875	-2.071962
H	0.856413	4.920017	-2.087128
H	1.478703	3.567683	-3.040357
H	1.792553	3.655050	-1.289624
C	2.143027	-2.324086	2.972188
C	1.262307	-3.565391	2.885134
H	1.634994	-4.106460	2.003997
C	1.527691	-4.452524	4.115473
H	1.170395	-3.958849	5.026491
H	2.594203	-4.665851	4.240717
H	0.990989	-5.402725	4.019105
C	-0.244870	-3.386742	2.679736
H	-0.670021	-4.348865	2.372299
H	-0.452390	-2.655546	1.892635
H	-0.754584	-3.084178	3.599608
C	3.473517	-2.469472	2.562285
H	3.781981	-3.418244	2.128779
C	4.395252	-1.443207	2.696046
H	5.418418	-1.584446	2.359723
C	4.011379	-0.233702	3.261797
H	2.362480	1.309070	-0.051383
H	4.741647	0.562213	3.380574
C	2.696118	-0.031060	3.686471
C	2.312229	1.286009	4.337035
H	1.245498	1.252931	4.574813
C	2.521543	2.477846	3.394047
H	3.566760	2.563539	3.073861
H	2.252689	3.409919	3.902875
H	1.876882	2.382482	2.513220
C	3.075789	1.477016	5.655234
H	4.153556	1.572727	5.482446
H	2.917171	0.628994	6.329735
H	2.734404	2.386750	6.160912
C	1.777748	-1.084625	3.517025
C	-3.750817	-1.520717	3.122424
H	-2.743092	-1.648128	2.705486
C	-4.749141	-1.939918	2.041775
H	-5.772551	-1.985799	2.431945
H	-4.493529	-2.939408	1.676173
H	-4.728200	-1.254012	1.190911
C	-3.894814	-2.445658	4.342188
H	-3.137789	-2.242877	5.104426
H	-3.790077	-3.492676	4.035973
H	-4.883267	-2.320154	4.799579
H	2.694230	0.403048	1.283617
H	3.074578	-0.210299	-0.204068
N	3.735160	-2.014575	-0.847218
H	3.793966	-2.009211	-1.861473
H	4.461717	-2.631556	-0.504003
H	2.837705	-2.431500	-0.602996

Calculated energies and coordinates of **TS[G-H]**

Electronic energy ... -4113.80297463 Eh
Total Enthalpy ... -4112.49989350 Eh
Final Gibbs free energy ... -4112.67887209 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.643129	-0.012116	-3.580963
Si	-0.574898	0.892829	-1.764575
Si	0.683553	0.210085	0.160341
P	-0.841822	0.793705	1.733994
Si	-2.727723	-0.098297	-1.713775
Si	-0.874138	3.228261	-2.016941
N	-1.453892	-0.312575	4.163198
N	0.548106	-0.990486	3.615590
N	2.007137	1.556094	0.254237
C	-0.283691	2.943099	-8.992967
H	-1.217585	2.625870	-9.467274
H	0.535452	2.775564	-9.698296
H	-0.355887	4.024295	-8.821283
C	-0.051434	2.211573	-7.699055
C	1.235975	1.863870	-7.287209
H	2.083550	2.102187	-7.926832
C	1.451378	1.214289	-6.074959
H	2.468340	0.953883	-5.790537
C	0.387348	0.890091	-5.223031
C	-0.506705	-0.209954	3.149823
C	-2.688597	0.415659	4.197519
C	-2.683094	1.706239	4.742492
C	-1.409304	2.374880	5.220103
H	-0.568605	1.721042	4.968455
C	-1.419688	2.556517	6.743882
H	-2.235937	3.217366	7.056878
H	-0.477259	3.001571	7.082666
H	-1.549443	1.597219	7.256628
C	-5.074907	1.781770	4.383272
H	-6.016829	2.318129	4.457402
C	-5.048238	0.508877	3.825683
H	-5.970360	0.068896	3.460182
C	-3.853258	-0.201268	3.715589
C	-3.904402	2.375741	4.831883
H	-3.936030	3.377548	5.251320
C	-1.172443	3.707548	4.498475
H	-1.182096	3.559538	3.413976
H	-0.198587	4.121488	4.785362
H	-1.936853	4.448345	4.758516
C	-0.995029	-1.100284	5.203829
H	-1.580509	-1.262187	6.094916
C	0.234084	-1.534251	4.864558
H	0.942645	-2.144882	5.400716
C	0.180197	-1.829595	-3.804377

C	-0.295397	-2.342684	-5.016392
H	-0.404095	-1.681039	-5.873519
C	-0.630359	-3.688110	-5.148447
H	-0.999704	-4.058835	-6.102554
C	-0.495580	-4.571196	-4.076325
C	-0.012011	-4.066572	-2.865144
H	0.097928	-4.735376	-2.012962
C	0.312208	-2.722460	-2.728999
H	0.661112	-2.351184	-1.763639
C	-0.888836	-6.017744	-4.206116
H	-1.910074	-6.177356	-3.838276
H	-0.227343	-6.664614	-3.621262
H	-0.859354	-6.347333	-5.248724
C	-1.119528	1.883340	-6.859654
H	-2.134383	2.139067	-7.158583
C	-0.901850	1.242702	-5.646058
H	-1.754010	1.010341	-5.012726
C	2.524761	0.013275	-3.289792
C	3.190848	1.210380	-2.986545
H	2.616891	2.127936	-2.877347
C	4.572023	1.263868	-2.836279
H	5.051636	2.211361	-2.598526
C	5.356081	0.115181	-2.989405
C	6.854131	0.178616	-2.864577
H	7.161647	0.898204	-2.099503
H	7.306830	0.497372	-3.811513
H	7.276971	-0.798221	-2.612312
C	4.704391	-1.083309	-3.297250
H	5.290640	-1.990881	-3.430280
C	3.317739	-1.131188	-3.448007
H	2.844626	-2.079675	-3.691705
C	-3.895394	0.994057	-0.701227
H	-3.988042	1.999514	-1.125032
H	-3.536635	1.092011	0.329911
H	-4.899432	0.550111	-0.682876
C	-2.667661	-1.804320	-0.908115
H	-3.677092	-2.232355	-0.868787
H	-2.281502	-1.729501	0.114547
H	-2.028247	-2.489656	-1.472934
C	-3.511074	-0.322013	-3.424606
H	-2.885748	-0.938755	-4.079982
H	-3.697720	0.637142	-3.920354
H	-4.478517	-0.828666	-3.313498
C	-2.245303	3.683588	-3.242912
H	-3.187467	3.170461	-3.025777
H	-1.950659	3.431364	-4.267001
H	-2.434723	4.764075	-3.202828
C	-1.304207	3.968059	-0.331189
H	-0.507049	3.774317	0.395340
H	-2.219602	3.530337	0.080381
H	-1.445581	5.053444	-0.411856
C	0.683950	4.109838	-2.648042
H	0.471184	5.178625	-2.778810
H	0.999284	3.713896	-3.620600
H	1.524331	4.031301	-1.948507
C	2.260423	-2.451650	2.666821
C	1.319686	-3.607810	2.335980
H	1.794712	-4.090111	1.468441
C	1.302299	-4.652149	3.465709
H	0.790311	-4.257416	4.349286
H	2.313244	-4.953802	3.758957
H	0.756566	-5.544587	3.140281
C	-0.106826	-3.253551	1.906264
H	-0.545001	-4.112966	1.386517
H	-0.118912	-2.396790	1.224322
H	-0.748605	-3.030396	2.764164
C	3.628134	-2.699558	2.506578
H	3.943020	-3.683912	2.165780
C	4.582109	-1.724681	2.773973
H	5.640209	-1.953263	2.673439
C	4.176532	-0.453102	3.169297
H	2.007178	2.142063	-0.575724
H	4.924546	0.309739	3.359806
C	2.827869	-0.152786	3.357835
C	2.405580	1.211527	3.873858
H	1.423431	1.437235	3.434661
C	3.364272	2.334394	3.462065
H	4.302333	2.296051	4.028167
H	2.900889	3.303426	3.675054
H	3.602604	2.295304	2.394531
C	2.261541	1.202301	5.405496
H	3.221084	0.957646	5.876637
H	1.517796	0.477275	5.747511
H	1.953757	2.193976	5.757022
C	1.880926	-1.175036	3.118845
C	-3.810544	-1.590445	3.108048
H	-2.817490	-1.714272	2.657440
C	-4.842635	-1.786435	1.995083
H	-5.864855	-1.816160	2.389014
H	-4.659820	-2.740299	1.490300
H	-4.776936	-0.989530	1.249710
C	-3.995058	-2.671088	4.185585
H	-3.221717	-2.616392	4.956745
H	-3.950606	-3.668685	3.734112
H	-4.970482	-2.559549	4.673576
H	1.795793	2.182341	1.026484
H	3.376260	0.390202	0.094500
N	3.572977	-0.638296	-0.109033
H	3.995218	-0.774800	-1.028344
H	4.107119	-1.081874	0.638100
H	2.524382	-0.961002	-0.095132

Calculated energies and coordinates of **H**

Electronic energy ... -4113.86291401 Eh
Total Enthalpy ... -4112.55936583 Eh
Final Gibbs free energy ... -4112.74338748 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.672752	0.092918	-3.630351
Si	-0.715427	0.816266	-1.851374
Si	0.570399	0.350248	0.099113
P	-0.955451	0.649916	1.692758
Si	-2.838239	-0.238226	-1.807846
Si	-1.050151	3.159569	-1.968256

N	-1.337765	-0.274400	4.232187
N	0.673452	-0.852174	3.630966
N	1.971279	1.394277	0.234432
C	-0.191592	3.102911	-9.009978
H	-1.158818	2.849225	-9.453851
H	0.593369	2.869593	-9.735321
H	-0.178938	4.188129	-8.849439
C	0.024148	2.369370	-7.714553
C	1.307065	2.012307	-7.294446
H	2.160555	2.243735	-7.928516
C	1.509042	1.360750	-6.081575
H	2.520860	1.088234	-5.789496
C	0.434960	1.044673	-5.238826
C	-0.445616	-0.185463	3.177912
C	-2.573498	0.450554	4.308622
C	-2.540092	1.746998	4.837620
C	-1.245729	2.420726	5.251307
H	-0.420393	1.725179	5.066237
C	-1.239228	2.754485	6.748466
H	-2.018619	3.483054	6.997821
H	-0.273934	3.185653	7.036060
H	-1.409841	1.859542	7.356381
C	-4.940253	1.834571	4.542848
H	-5.876027	2.378512	4.636301
C	-4.938860	0.555219	3.998240
H	-5.873635	0.118800	3.662028
C	-3.752699	-0.164628	3.863081
C	-3.754482	2.426308	4.951738
H	-3.767419	3.434269	5.356970
C	-0.979781	3.668986	4.398495
H	-0.986935	3.412581	3.334237
H	-0.000510	4.092736	4.649889
H	-1.735779	4.442361	4.575011
C	-0.775402	-0.954925	5.299855
H	-1.309259	-1.094628	6.226310
C	0.465833	-1.323692	4.924610
H	1.237714	-1.860062	5.452120
C	0.337879	-1.735166	-3.967828
C	0.264268	-2.239515	-5.272980
H	0.396467	-1.565554	-6.116846
C	0.021972	-3.588168	-5.513201
H	-0.028837	-3.950525	-6.538021
C	-0.159815	-4.486799	-4.459593
C	-0.088048	-3.992142	-3.154943
H	-0.232619	-4.670019	-2.315087
C	0.153076	-2.642897	-2.916051
H	0.190213	-2.289269	-1.886447
C	-0.460479	-5.937268	-4.721289
H	-1.540919	-6.096870	-4.824431
H	-0.112364	-6.571154	-3.900391
H	0.010948	-6.280641	-5.646947
C	-1.052928	2.044773	-6.885755
H	-2.063702	2.303327	-7.195190
C	-0.849069	1.398690	-5.672617
H	-1.708521	1.158753	-5.050932
C	2.469737	0.285220	-3.069777
C	3.114240	1.530993	-3.065578
H	2.625767	2.394244	-3.509518
C	4.369849	1.696101	-2.490102
H	4.840146	2.677443	-2.500464
C	5.030765	0.623846	-1.882657
C	6.350427	0.817759	-1.188569
H	6.193804	1.060112	-0.129405
H	6.920907	1.638722	-1.632740
H	6.960711	-0.089446	-1.230574
C	4.410077	-0.626092	-1.911800
H	4.909047	-1.482113	-1.461828
C	3.160196	-0.791012	-2.498875
H	2.711607	-1.780692	-2.512939
C	-4.041304	0.824515	-0.807533
H	-4.171450	1.824721	-1.232731
H	-3.685646	0.937474	0.223106
H	-5.027460	0.342662	-0.782049
C	-2.792895	-1.940320	-0.991091
H	-3.817493	-2.321738	-0.894969
H	-2.359162	-1.872966	0.013154
H	-2.217813	-2.662731	-1.577254
C	-3.533563	-0.450384	-3.554797
H	-2.848136	-1.022022	-4.191208
H	-3.725262	0.514876	-4.036810
H	-4.486280	-0.993447	-3.513449
C	-2.423547	3.618719	-3.187589
H	-3.342383	3.046731	-3.025927
H	-2.098392	3.454314	-4.220072
H	-2.668352	4.682885	-3.078576
C	-1.518865	3.829437	-0.264810
H	-0.736924	3.628302	0.475825
H	-2.437679	3.371432	0.115725
H	-1.671976	4.914861	-0.319912
C	0.501909	4.070650	-2.549116
H	0.325334	5.153538	-2.527175
H	0.751256	3.793399	-3.579800
H	1.369857	3.856535	-1.916544
C	2.249949	-2.293394	2.437850
C	1.332950	-3.510666	2.378406
H	1.678125	-4.062858	1.494314
C	1.563636	-4.436179	3.585627
H	1.188737	-3.982315	4.508958
H	2.626431	-4.661940	3.718958
H	1.027131	-5.380324	3.439834
C	-0.165287	-3.259199	2.172468
H	-0.632160	-4.182976	1.812896
H	-0.354392	-2.474882	1.433050
H	-0.672276	-2.982821	3.102702
C	3.539970	-2.464010	1.924079
H	3.806134	-3.431888	1.505939
C	4.465129	-1.432330	1.938244
H	5.460134	-1.589515	1.529880
C	4.123447	-0.194978	2.465783
H	2.679525	1.258519	-0.480853
H	4.851774	0.608187	2.455551
C	2.856596	0.033355	2.998730
C	2.494794	1.378815	3.608067
H	1.463196	1.603530	3.303750
C	3.374422	2.529508	3.111652
H	4.385852	2.475572	3.532072

H	2.941488	3.481757	3.436087
H	3.443476	2.532446	2.021417
C	2.556941	1.336525	5.145339
H	3.571416	1.086118	5.477283
H	1.867208	0.605897	5.574832
H	2.300577	2.320465	5.555811
C	1.937162	-1.033779	2.971631
C	-3.727628	-1.559490	3.267591
H	-2.758773	-1.676995	2.765866
C	-4.811526	-1.776562	2.209524
H	-5.812854	-1.816680	2.653047
H	-4.641801	-2.730976	1.700932
H	-4.793623	-0.982879	1.457298
C	-3.839713	-2.627935	4.366198
H	-3.027674	-2.551299	5.095459
H	-3.802606	-3.630619	3.925858
H	-4.789643	-2.524261	4.903481
H	1.750092	2.382112	0.280331
H	2.551197	-3.178536	-0.642398
N	2.738188	-4.128113	-0.955422
H	2.253202	-4.225116	-1.842948
H	3.729195	-4.154058	-1.174811
H	1.135307	-1.027596	-0.037607

Calculated energies and coordinates of **I**

Electronic energy ... -4113.81057979 Eh
Total Enthalpy ... -4112.50446237 Eh
Final Gibbs free energy ... -4112.68754869 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.768924	-0.420281	-3.544947
Si	-0.720084	0.381266	-1.860781
Si	0.099868	0.044464	0.387874
P	-1.221114	1.084097	1.842263
Si	-2.834377	-0.686192	-2.031339
Si	-1.090935	2.714436	-2.210292
N	-1.549757	-0.028717	4.378473
N	0.342632	-0.675816	3.498281
N	1.670098	1.143113	0.252138
C	0.196713	2.855657	-8.816818
H	-0.577699	2.436282	-9.466550
H	1.134115	2.895580	-9.378780
H	-0.094968	3.887729	-8.586080
C	0.347254	2.050258	-7.555594
C	1.596915	1.858032	-6.965162
H	2.482303	2.273511	-7.441948
C	1.730317	1.137115	-5.781723
H	2.722389	0.997762	-5.359465
C	0.615790	0.586372	-5.136104
C	-0.769388	0.086336	3.248285
C	-2.717474	0.759410	4.647297
C	-2.546841	1.980789	5.311724
C	-1.177082	2.527944	5.666850
H	-0.419688	1.817187	5.318695
C	-1.010067	2.676910	7.184748
H	-1.716382	3.408550	7.592538
H	0.002564	3.019743	7.423919
H	-1.180243	1.724442	7.697761
C	-4.952591	2.243665	5.271905
H	-5.835597	2.824955	5.522598
C	-5.089614	1.043801	4.582548
H	-6.079020	0.706240	4.291583
C	-3.973936	0.277828	4.248919
C	-3.695716	2.711120	5.624545
H	-3.601254	3.661975	6.141708
C	-0.915048	3.855818	4.942804
H	-1.028143	3.731568	3.861256
H	0.104378	4.201536	5.148367
H	-1.608230	4.636031	5.276653
C	-0.905657	-0.813524	5.323810
H	-1.338747	-0.997183	6.294444
C	0.252219	-1.237760	4.766946
H	1.019007	-1.895930	5.142727
C	0.350131	-2.217324	-3.928894
C	0.035340	-2.660368	-5.218842
H	0.022343	-1.951425	-6.043696
C	-0.256283	-3.998914	-5.468633
H	-0.499115	-4.314830	-6.481059
C	-0.233653	-4.945583	-4.443154
C	0.090850	-4.511526	-3.154215
H	0.115938	-5.228211	-2.335524
C	0.366322	-3.173941	-2.904448
H	0.593436	-2.865095	-1.885575
C	-0.575436	-6.386587	-4.706150
H	-0.436527	-6.643524	-5.760066
H	-1.622813	-6.590007	-4.450986
H	0.042762	-7.058329	-4.102559
C	-0.767653	1.487757	-6.927496
H	-1.753167	1.612291	-7.372321
C	-0.634351	0.776743	-5.741632
H	-1.523712	0.356052	-5.279660
C	2.583387	-0.338236	-3.016497
C	3.179873	0.891197	-2.695982
H	2.596000	1.808045	-2.757656
C	4.518273	0.976191	-2.328222
H	4.947708	1.948353	-2.097429
C	5.317522	-0.167272	-2.260346
C	6.745431	-0.084276	-1.797746
H	7.202144	0.869758	-2.078363
H	7.350086	-0.893575	-2.216931
H	6.800634	-0.165861	-0.704231
C	4.738490	-1.390454	-2.602241
H	5.344187	-2.294027	-2.573652
C	3.400578	-1.474684	-2.974230
H	2.985877	-2.444582	-3.238546
C	-4.034843	0.249703	-0.915044
H	-4.200440	1.274116	-1.266196
H	-3.646022	0.308933	0.108305
H	-5.006397	-0.260119	-0.891498
C	-2.787743	-2.497545	-1.506112
H	-3.815282	-2.868140	-1.397715
H	-2.273008	-2.648605	-0.554355
H	-2.283826	-3.106906	-2.262853
C	-3.515781	-0.685741	-3.795852

H	-2.888861	-1.294288	-4.457838
H	-3.608109	0.318089	-4.221727
H	-4.516571	-1.136645	-3.785539
C	-2.420829	3.023871	-3.519428
H	-3.379707	2.575561	-3.240205
H	-2.129495	2.637336	-4.500172
H	-2.575810	4.106270	-3.616137
C	-1.675033	3.579107	-0.637245
H	-1.904163	4.626585	-0.872898
H	-0.921914	3.567725	0.157692
H	-2.576813	3.117244	-0.222705
C	0.476220	3.603465	-2.791806
H	0.238725	4.659003	-2.976098
H	0.859251	3.179211	-3.726612
H	1.277431	3.580273	-2.043627
C	1.116998	-1.452379	1.256111
C	0.332540	-2.804098	1.299943
H	0.257457	-3.111441	0.244583
C	1.148185	-3.868653	2.040065
H	1.262736	-3.592245	3.095233
H	2.151592	-3.966389	1.614825
H	0.644812	-4.841200	1.996767
C	-1.095844	-2.767120	1.849981
H	-1.627165	-3.683138	1.566160
H	-1.659114	-1.912576	1.457771
H	-1.110666	-2.712405	2.943800
C	2.394866	-1.652695	0.486394
H	2.319220	-2.202650	-0.448962
C	3.606293	-1.184792	0.888914
H	4.466979	-1.379521	0.251145
C	3.786340	-0.451925	2.091552
H	2.276509	0.875985	-0.529537
H	4.775245	-0.131246	2.400367
C	2.687673	-0.319344	2.958940
C	2.891140	0.420009	4.275947
H	1.928036	0.507234	4.788650
C	3.391005	1.853186	4.047183
H	4.389119	1.859226	3.596389
H	3.449660	2.391840	5.000625
H	2.708728	2.403009	3.388260
C	3.844619	-0.343634	5.204615
H	4.849146	-0.401146	4.772901
H	3.500562	-1.370433	5.367587
H	3.919808	0.154781	6.178182
C	1.442963	-0.835928	2.598304
C	-4.099206	-1.029714	3.492906
H	-3.199170	-1.125519	2.875357
C	-5.301821	-1.063559	2.546776
H	-6.249404	-1.141088	3.092281
H	-5.229209	-1.939960	1.893976
H	-5.336481	-0.171703	1.914027
C	-4.146440	-2.223322	4.459310
H	-3.251706	-2.270692	5.087194
H	-4.213855	-3.162496	3.898813
H	-5.021830	-2.150967	5.115464
H	1.464758	2.136404	0.171249
H	2.239728	1.019174	1.100363
N	4.235507	2.887162	0.695481
H	5.002647	3.160478	0.090643
H	4.335500	3.439728	1.540801
H	4.417688	1.922862	0.973842

Calculated energies and coordinates of **TS[I-J]**

Electronic energy ... -4113.79644857 Eh
Total Enthalpy ... -4112.49594368 Eh
Final Gibbs free energy ... -4112.67246289 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.883726	-0.391827	-3.501261
Si	-0.721214	0.305049	-1.857680
Si	0.166829	0.408870	0.401337
P	-1.172878	1.398790	1.880877
Si	-2.692469	-1.000544	-2.088654
Si	-1.345540	2.571602	-2.331782
N	-1.581826	0.188367	4.344374
N	0.307293	-0.503572	3.478993
N	1.498397	1.641681	0.066980
C	-0.049956	2.613430	-8.881901
H	-0.954870	2.260124	-9.385107
H	0.794415	2.496798	-9.567563
H	-0.176556	3.687094	-8.695354
C	0.183664	1.872746	-7.593901
C	1.475021	1.664429	-7.105710
H	2.327117	2.018436	-7.682526
C	1.690224	1.006288	-5.898741
H	2.710864	0.855417	-5.555804
C	0.619864	0.536158	-5.126322
C	-0.762444	0.325609	3.240130
C	-2.694773	1.039973	4.647092
C	-2.442396	2.224541	5.351348
C	-1.038912	2.664334	5.722607
H	-0.329644	1.935530	5.316139
C	-0.851801	2.695384	7.245543
H	-1.511732	3.435421	7.711958
H	0.180998	2.960615	7.497134
H	-1.073876	1.719866	7.690811
C	-4.826935	2.636951	5.353351
H	-5.669250	3.262769	5.635023
C	-5.046096	1.469820	4.630883
H	-6.058464	1.201834	4.346675
C	-3.983903	0.647600	4.257254
C	-3.539196	3.013686	5.703531
H	-3.379817	3.936856	6.253819
C	-0.702446	4.021358	5.090019
H	-0.830991	3.978565	4.004056
H	0.337325	4.290642	5.307673
H	-1.343621	4.817340	5.484839
C	-1.023253	-0.701113	5.246888
H	-1.496939	-0.924436	6.189673
C	0.121504	-1.160486	4.694072
H	0.812999	-1.912324	5.036173
C	0.633435	-2.233818	-3.839396
C	0.105212	-2.674002	-5.059961
H	-0.110426	-1.952989	-5.845095

C	-0.147900	-4.022577	-5.295811
H	-0.561464	-4.329743	-6.254124
C	0.127173	-4.987898	-4.326869
C	0.668451	-4.559331	-3.111711
H	0.893408	-5.288764	-2.336101
C	0.905297	-3.212559	-2.870811
H	1.301492	-2.928072	-1.899127
C	-0.175346	-6.441735	-4.564775
H	-0.260605	-6.662392	-5.632475
H	-1.124036	-6.722321	-4.090757
H	0.602476	-7.084166	-4.140263
C	-0.887919	1.391502	-6.837679
H	-1.904814	1.530005	-7.200132
C	-0.671022	0.742491	-5.628356
H	-1.526602	0.385325	-5.061888
C	2.690379	-0.069806	-3.017115
C	3.147518	1.243323	-2.840603
H	2.473144	2.077808	-3.027487
C	4.463030	1.517201	-2.471531
H	4.786557	2.551547	-2.363254
C	5.378773	0.482912	-2.267056
C	6.797047	0.759627	-1.846621
H	6.986364	1.833206	-1.756248
H	7.510064	0.352460	-2.571910
H	7.021323	0.290018	-0.881031
C	4.940942	-0.827606	-2.478731
H	5.641367	-1.650848	-2.351482
C	3.630097	-1.097096	-2.851217
H	3.333236	-2.129821	-3.016201
C	-3.934765	-0.292992	-0.854295
H	-4.256576	0.711694	-1.152113
H	-3.499690	-0.205625	0.147622
H	-4.827568	-0.927559	-0.794048
C	-2.451612	-2.847061	-1.790033
H	-3.437916	-3.328606	-1.761623
H	-1.936049	-3.078042	-0.856603
H	-1.881323	-3.293046	-2.611440
C	-3.463793	-0.920885	-3.816914
H	-2.825793	-1.418175	-4.556397
H	-3.677932	0.094453	-4.161234
H	-4.414808	-1.468987	-3.788173
C	-2.805351	2.740124	-3.527127
H	-3.699860	2.234886	-3.148948
H	-2.589162	2.363092	-4.529762
H	-3.043969	3.807769	-3.617321
C	-1.905239	3.491064	-0.778998
H	-2.233710	4.497317	-1.070623
H	-1.116529	3.602080	-0.028007
H	-2.742292	2.991055	-0.281072
C	0.083153	3.575658	-3.068707
H	-0.280201	4.583148	-3.308459
H	0.469896	3.130801	-3.991818
H	0.912902	3.693017	-2.361824
C	1.059842	-1.132553	1.181449
C	0.211369	-2.454910	1.094653
H	0.152052	-2.669824	0.015277
C	0.952266	-3.612949	1.766758
H	1.025056	-3.440868	2.847811
H	1.969891	-3.712568	1.377643
H	0.418137	-4.557395	1.611250
C	-1.228412	-2.388433	1.614996
H	-1.774646	-3.292673	1.321618
H	-1.769603	-1.522327	1.216575
H	-1.264167	-2.339465	2.708340
C	2.334643	-1.331594	0.387115
H	2.221412	-1.533542	-0.673326
C	3.571057	-1.366089	0.941879
H	4.418120	-1.598509	0.294957
C	3.817916	-1.009553	2.297236
H	1.778599	1.600755	-0.914421
H	4.802011	-1.145387	2.733411
C	2.705215	-0.687732	3.118596
C	3.006598	-0.211220	4.536867
H	2.071711	0.066288	5.032666
C	3.872079	1.057962	4.526296
H	4.850315	0.870965	4.070312
H	4.038577	1.414662	5.549722
H	3.370010	1.858417	3.970639
C	3.678076	-1.305779	5.377557
H	4.673057	-1.544760	4.988778
H	3.097143	-2.234185	5.366730
H	3.791225	-0.980601	6.418371
C	1.421123	-0.724488	2.606157
C	-4.205353	-0.631398	3.474641
H	-3.308463	-0.792394	2.865251
C	-5.398549	-0.548326	2.520251
H	-6.352647	-0.535091	3.059372
H	-5.406557	-1.426683	1.866948
H	-5.341555	0.342699	1.887593
C	-4.364939	-1.833078	4.419336
H	-3.484968	-1.967765	5.054870
H	-4.506162	-2.753277	3.841455
H	-5.238405	-1.697081	5.067903
H	1.089875	2.563292	0.219835
H	2.740706	1.632891	0.688324
N	3.901222	1.625286	1.061651
H	4.490095	1.538564	0.235685
H	4.178522	2.443163	1.594172
H	4.019600	0.740820	1.643589

Calculated energies and coordinates of **J**

Electronic energy ... -4113.84770203 Eh
Total Enthalpy ... -4112.54130619 Eh
Final Gibbs free energy ... -4112.72225023 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Si	0.884044	-0.467486	-3.449707
Si	-0.674874	0.282174	-1.787246
Si	0.249011	0.437154	0.435204
P	-1.244378	1.267114	1.883330
Si	-2.687533	-0.964364	-2.045607
Si	-1.215292	2.579919	-2.237123
N	-1.656762	0.021306	4.330192
N	0.205184	-0.680339	3.441398

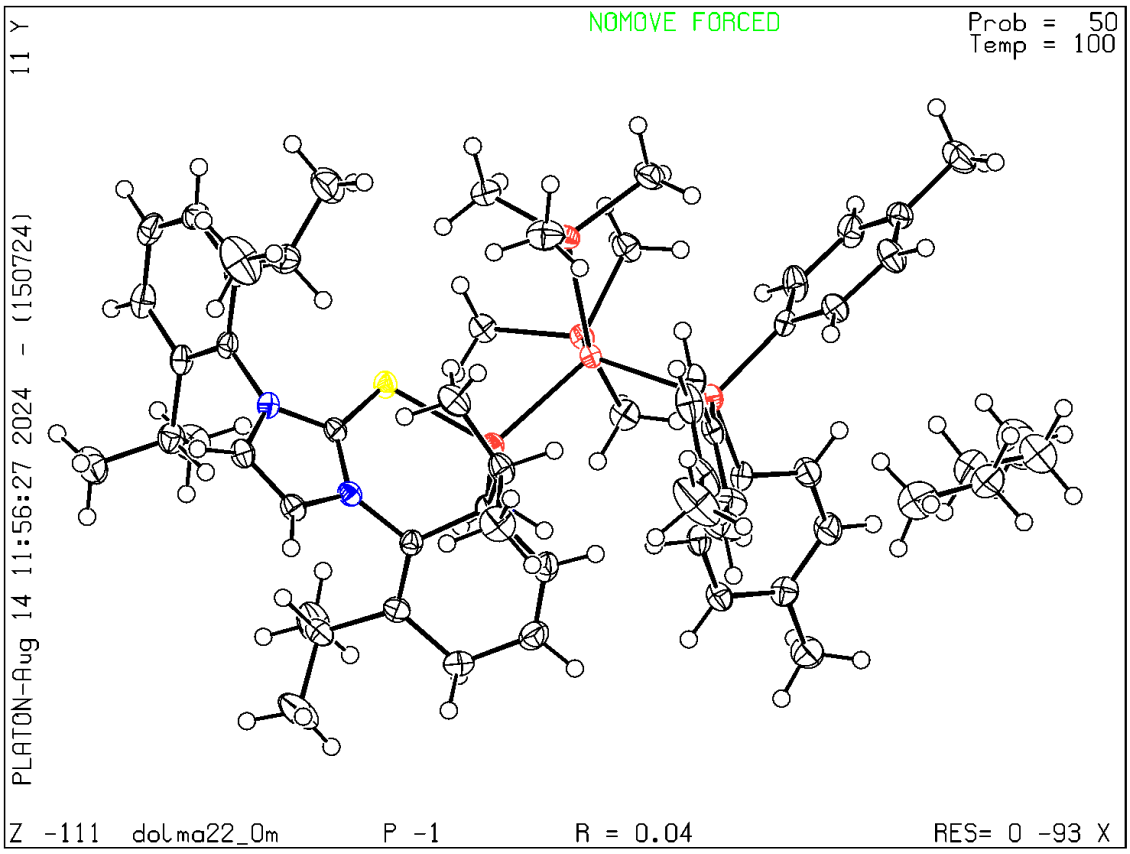
N	1.595198	1.568107	0.321930
C	0.060667	2.665628	-8.774968
H	-0.842761	2.339070	-9.298854
H	0.912374	2.551645	-9.451768
H	-0.052229	3.736330	-8.564322
C	0.264475	1.890993	-7.501921
C	1.546270	1.609490	-7.025587
H	2.411997	1.931379	-7.600807
C	1.734867	0.921438	-5.830842
H	2.748296	0.717688	-5.493984
C	0.646353	0.492047	-5.060413
C	-0.851212	0.172009	3.218493
C	-2.746886	0.891743	4.661239
C	-2.455501	2.067116	5.365953
C	-1.036258	2.472415	5.716196
H	-0.348311	1.746201	5.269726
C	-0.812929	2.449365	7.234524
H	-1.452222	3.181999	7.739790
H	0.229158	2.692867	7.469214
H	-1.038086	1.462587	7.652838
C	-4.830824	2.528477	5.406197
H	-5.655013	3.170553	5.704259
C	-5.086905	1.372119	4.678418
H	-6.108840	1.129727	4.405756
C	-4.048119	0.530066	4.283575
C	-3.530199	2.876476	5.739103
H	-3.343439	3.793533	6.290879
C	-0.687103	3.842668	5.120912
H	-0.854963	3.844669	4.039502
H	0.367429	4.074118	5.307808
H	-1.289561	4.640715	5.568901
C	-1.101712	-0.898429	5.210063
H	-1.574891	-1.140289	6.148299
C	0.039050	-1.351093	4.647565
H	0.748923	-2.091486	4.980553
C	0.560716	-2.294561	-3.816162
C	-0.038291	-2.690332	-5.019160
H	-0.268203	-1.944277	-5.776395
C	-0.341441	-4.024807	-5.274843
H	-0.808412	-4.295874	-6.219422
C	-0.048397	-5.022023	-4.344067
C	0.565716	-4.639623	-3.148348
H	0.812128	-5.395918	-2.405613
C	0.854366	-3.306359	-2.889276
H	1.317822	-3.057841	-1.937849
C	-0.404259	-6.460115	-4.602634
H	-0.527907	-6.654272	-5.671717
H	-1.347634	-6.720890	-4.107076
H	0.364509	-7.136190	-4.215662
C	-0.825910	1.452175	-6.746824
H	-1.836611	1.649910	-7.099111
C	-0.635146	0.771929	-5.550410
H	-1.504427	0.451126	-4.983671
C	2.701617	-0.229807	-2.981473
C	3.188044	1.064644	-2.750291
H	2.515135	1.914836	-2.841031
C	4.525650	1.297133	-2.449285
H	4.871871	2.318005	-2.299264
C	5.433636	0.239646	-2.353640
C	6.867800	0.477762	-1.967854
H	7.175272	1.505157	-2.183944
H	7.541571	-0.202368	-2.497787
H	7.015006	0.308746	-0.893114
C	4.962806	-1.050078	-2.609039
H	5.655482	-1.888608	-2.569262
C	3.627117	-1.279415	-2.924068
H	3.305705	-2.295247	-3.141180
C	-3.926097	-0.290193	-0.789279
H	-4.159977	0.760572	-0.996300
H	-3.533444	-0.330809	0.232017
H	-4.863599	-0.858888	-0.829719
C	-2.493008	-2.831896	-1.840957
H	-3.490671	-3.284411	-1.768804
H	-1.923822	-3.128332	-0.959287
H	-1.993593	-3.252967	-2.719625
C	-3.471069	-0.802621	-3.763828
H	-2.854258	-1.289644	-4.527394
H	-3.668086	0.227363	-4.072162
H	-4.433050	-1.331644	-3.740014
C	-2.691771	2.806852	-3.401721
H	-3.596643	2.332821	-3.007735
H	-2.511004	2.429910	-4.411350
H	-2.892625	3.883171	-3.480564
C	-1.711659	3.513592	-0.671363
H	-1.975990	4.541112	-0.953775
H	-0.910712	3.566141	0.072298
H	-2.578650	3.064638	-0.176456
C	0.243868	3.523624	-2.984210
H	-0.071189	4.552245	-3.201460
H	0.598863	3.075472	-3.918011
H	1.081203	3.579880	-2.279446
C	1.052407	-1.198830	1.172389
C	0.203189	-2.500906	0.999900
H	0.138518	-2.640991	-0.089679
C	0.942053	-3.707555	1.588708
H	1.017733	-3.614043	2.679451
H	1.958226	-3.793803	1.191640
H	0.400721	-4.634903	1.370811
C	-1.238745	-2.479459	1.519164
H	-1.762048	-3.375195	1.166790
H	-1.788992	-1.602718	1.163876
H	-1.287264	-2.497226	2.612305
C	2.323206	-1.356625	0.396341
H	2.212816	-1.652692	-0.644172
C	3.545151	-1.140575	0.874733
H	4.404172	-1.264750	0.216811
C	3.808978	-0.723158	2.283366
H	2.193456	1.470902	-0.492850
H	4.428199	-1.487675	2.784346
C	2.562774	-0.497432	3.094668
C	2.759984	0.190923	4.433344
H	1.851075	0.085553	5.032519
C	2.966737	1.700733	4.208703
H	3.885149	1.902767	3.647559
H	3.039565	2.213273	5.175470
H	2.124927	2.124594	3.650468

C	3.915859	-0.403573	5.246387
H	4.881863	-0.229094	4.761029
H	3.795211	-1.484180	5.385354
H	3.956103	0.063445	6.236155
C	1.354592	-0.818123	2.596403
C	-4.305849	-0.736271	3.490495
H	-3.416635	-0.915552	2.873382
C	-5.502696	-0.613932	2.544353
H	-6.452055	-0.581550	3.090756
H	-5.537801	-1.485431	1.882838
H	-5.427448	0.281538	1.920141
C	-4.490491	-1.941212	4.426441
H	-3.611820	-2.101739	5.057896
H	-4.656911	-2.853621	3.843005
H	-5.357336	-1.788767	5.079975
H	1.322544	2.537952	0.426628
H	3.797877	2.164284	1.097530
N	4.807403	2.290353	1.036252
H	5.071409	1.859019	0.155572
H	4.972122	3.285507	0.927272
H	4.429672	0.185388	2.290826

Crystalographic Details

Data were collected on a single crystal X-ray diffractometer equipped with a CPAD detector (Bruker Photon-II), a TXS rotating anode with MoKα radiation (λ = 0.71073 Å) and a Helios optic using the APEX4 software package.[16] The crystal was fixed on the top of a kapton micro sampler with perfluorinated ether and transferred to the diffractometer, and frozen under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were corrected for Lorentz and polarisation effects, scan speed, and background using SAINT.[17] Absorption correction, including odd and even ordered spherical harmonics was performed using SADABS.[18] Space group assignment was based upon systematic absences, E statistics, and successful refinement of the structure. The structures were solved using SHELXT with the aid of successive difference Fourier maps and were refined against all data using SHELXL in conjunction with SHELXLE.[18-20] Hydrogen atoms (except on heteroatoms) were calculated in ideal positions as follows: Methyl hydrogen atoms were refined as part of rigid rotating groups, with a C–H distance of 0.98 Å and Uiso(H) = 1.5·U_{eq}(C). Non-methyl H atoms were placed in calculated positions and refined using a riding model with methylene, aromatic, and other C–H distances of 0.99 Å, 0.95 Å, and 1.00 Å, respectively, and Uiso(H) = 1.2·U_{eq}(C). Non-hydrogen atoms were refined with anisotropic displacement parameters. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2-F_c^2)^2$ with the SHELXL weighting scheme. Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[21] Images of the crystal structure were generated with Mercury and PLATON.[22, 23] Deposition Number 2377544 contains the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.

Compound **2** (CCDC = 2377544)



Supplementary Figure 11: PLATON generated image of compound **2**.

Diffractometer operator J.Y. Liu
scanspeed 8s per frame dx 41 mm
1779 frames measured in 6 data sets
phi-scans with delta_phi = 0.5
omega-scans with delta_omega = 0.5
shutterless mode

Crystal data

$C_{54}H_{78}N_3PSi_5 \cdot C_5H_{12}$	$F(000) = 1100$
$M_r = 1012.76$	
Triclinic, *P*	$D_x = 1.117$ Mg m^{-3}
Hall symbol: -P 1	
$a = 13.1621\ (7)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 13.9425\ (8)$ Å	Cell parameters from 9737 reflections
$c = 17.0349\ (10)$ Å	$\theta = 2.4–25.7°$
$\alpha = 93.904\ (2)°$	$\mu = 0.18$ mm^{-1}

β = 102.733 (2)°	T = 100 K
γ = 96.997 (2)°	Fragment, colorless
V = 3012.0 (3) Å^3	0.23 × 0.19 × 0.18 mm
Z = 2	

Data collection

Bruker Photon CMOS diffractometer	11227 independent reflections
Radiation source: TXS rotating anode	8755 reflections with $I > 2\sigma(I)$
Helios optic monochromator	R_{int} = 0.099
Detector resolution: 16 pixels mm^{-1}	θ_{max} = 25.7°, θ_{min} = 2.3°
phi– and ω–rotation scans	h = −16 16
Absorption correction: multi-scan *SADABS* 2016/2, Bruker, 2016	k = −17 17
T_{min} = 0.639, T_{max} = 0.745	l = −20 20
69338 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.114	W = 1/[$\Sigma^2(FO^2)$ + (0.0561P)^2 + 7.2754P] WHERE P = (FO^2 + 2FC^2)/3
S = 0.74	$(\Delta/\sigma)_{max}$ = 0.001
11227 reflections	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
638 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
0 restraints	Extinction correction: -
0 constraints	Extinction coefficient: -
Primary atom site location: iterative	

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