Tetrakis(ethylmethylamido) Hafnium Adsorption and Reaction on Hydrogen-Terminated Si(100) Surfaces

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Supporting Information

Supporting Information Figures: Pressure Drop vs. Time for TEMAH Gas in a Close Gas Cell Mode at Different Temperatures; Integrated Peak Area as a Function of Exposure Time of TEMAH to Ge for C-H Stretch, 1640, and 1600 cm^{-1}; Binding Energies of Si 2p for H-Si(100), Cleaned Si Wafer with Native Oxide, and Sputtered Si Substrate; Binding Energies of N 1s and C 1s of TEMAH Adsorption on H-Si(100) at 200°C with a Partial Pressure at 0.002 Torr; Gas Phase TEMAH reaction energies calculated at the B3LYP/BS1 level; Surface Reaction energies of TEMAH on H-Si(100) at the B3LYP/BS1 Level; Reaction Path of TEI-4 Chemisorption onto H-Si(100 Calculated at the B3LYP/BS1 Level; Average Thickness of the Adlayer as a Function of Substrate Temperature; and Cartesian Coordinates for the Bond Dissociation Energies Calculated at the B3LYP/BS2 Level.

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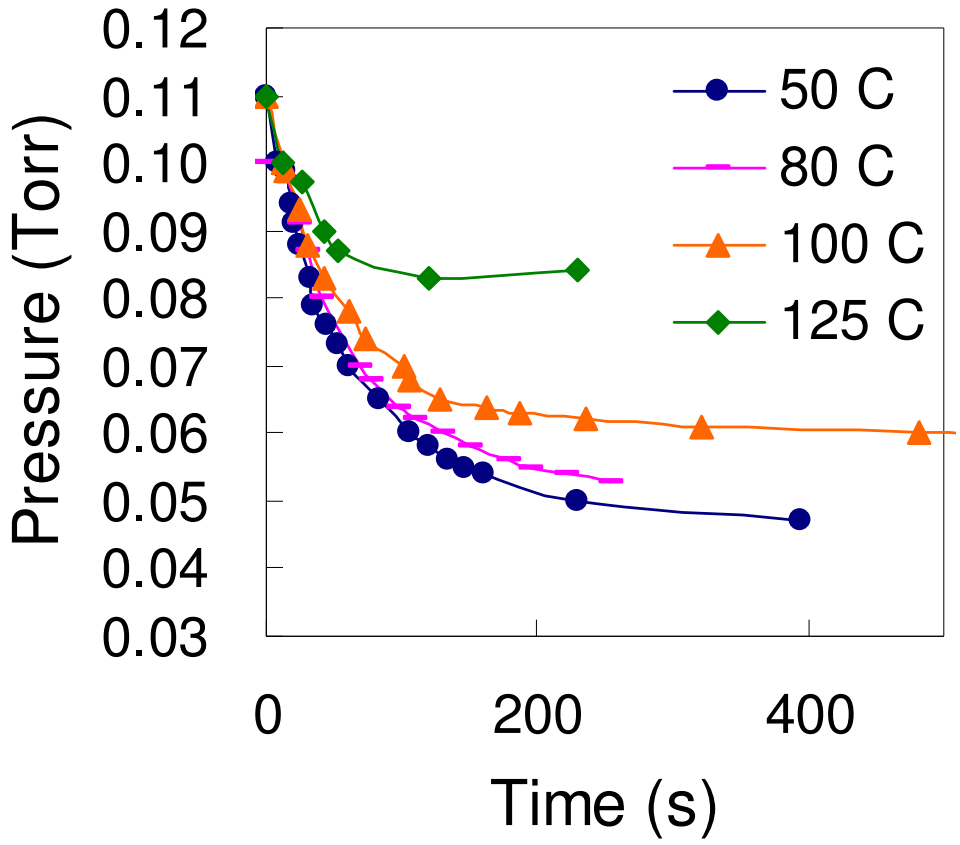


Figure S1. Pressure drop vs. time for TEMAH gas in a close gas cell mode at different temperatures.

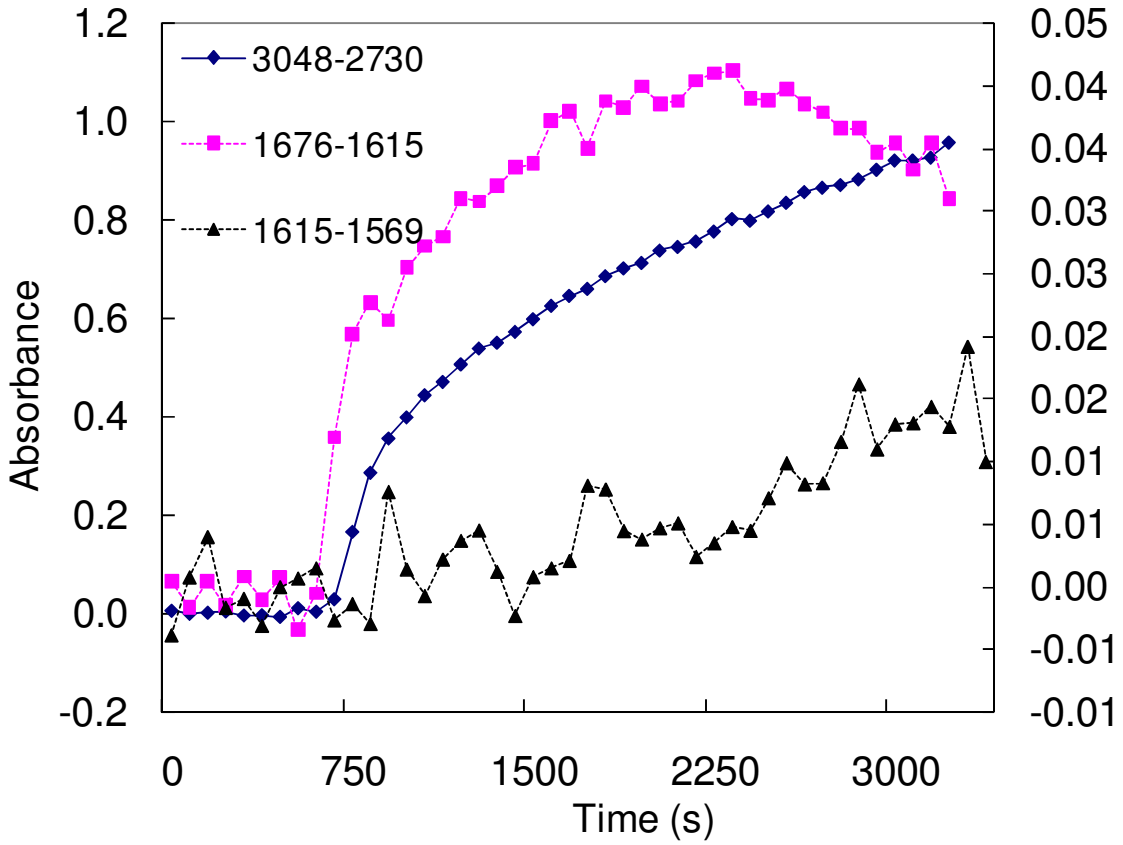


Figure S2. Integrated peak area as a function of exposure time of TEMAH to Ge for C-H stretch, 1640, and 1600 cm^{-1}. The C-H stretch region 3048-2730 cm^{-1} is to the left axis, and the other two to the right axis.

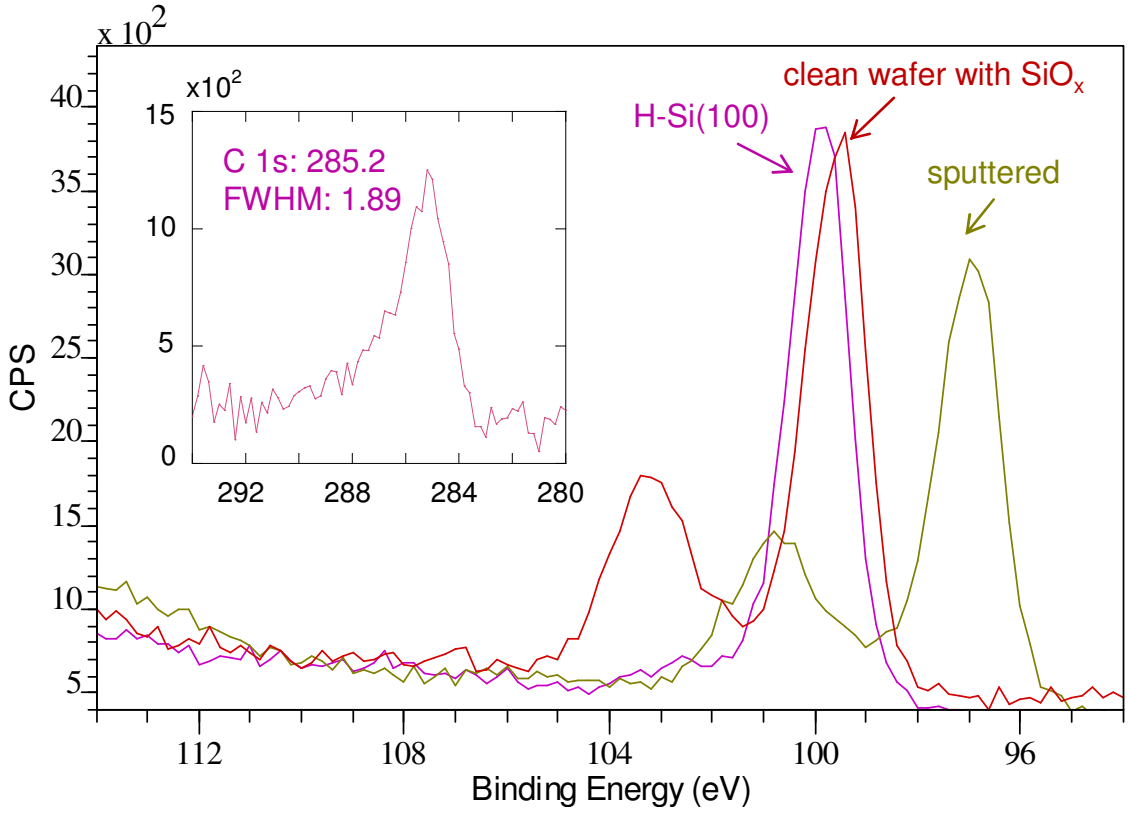


Figure S3. Binding energies of Si 2p for H-Si(100), cleaned Si wafer with native oxide, and sputtered Si substrate. The BE locates at 99.8 eV, 99.47 eV, 97.1 eV, respectively. Inset: C 1s spectrum of adventitious C on H-Si(100).

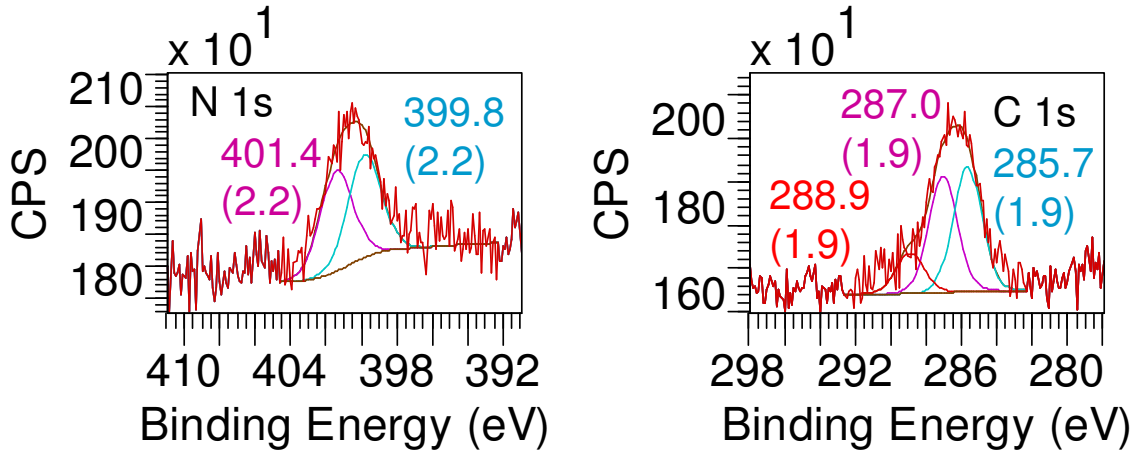


Figure S4. Binding energies of N 1s and C 1s of TEMAH adsorption on H-Si(100) at 200°C with a partial pressure at 0.002 Torr. The peak location and FWHM of each deconvoluted peak component are given in the same color.

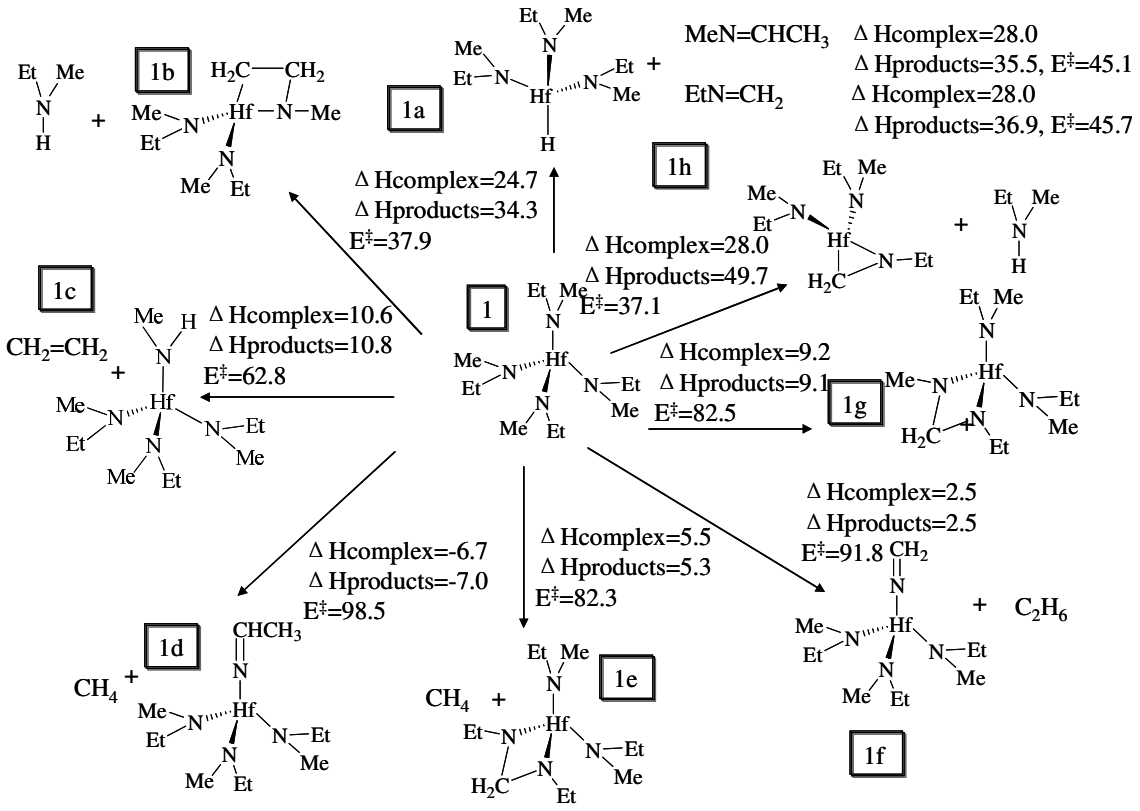


Figure S5. Gas phase TEMAH reactions ΔH_s is the total reaction energy; ΔH_c is the reaction energy to generate product complex; $E^{\ddagger}$ is the activation barrier; all at 0 K, and in kcal/mol. The calculations were performed at the B3LYP/BS1 level.

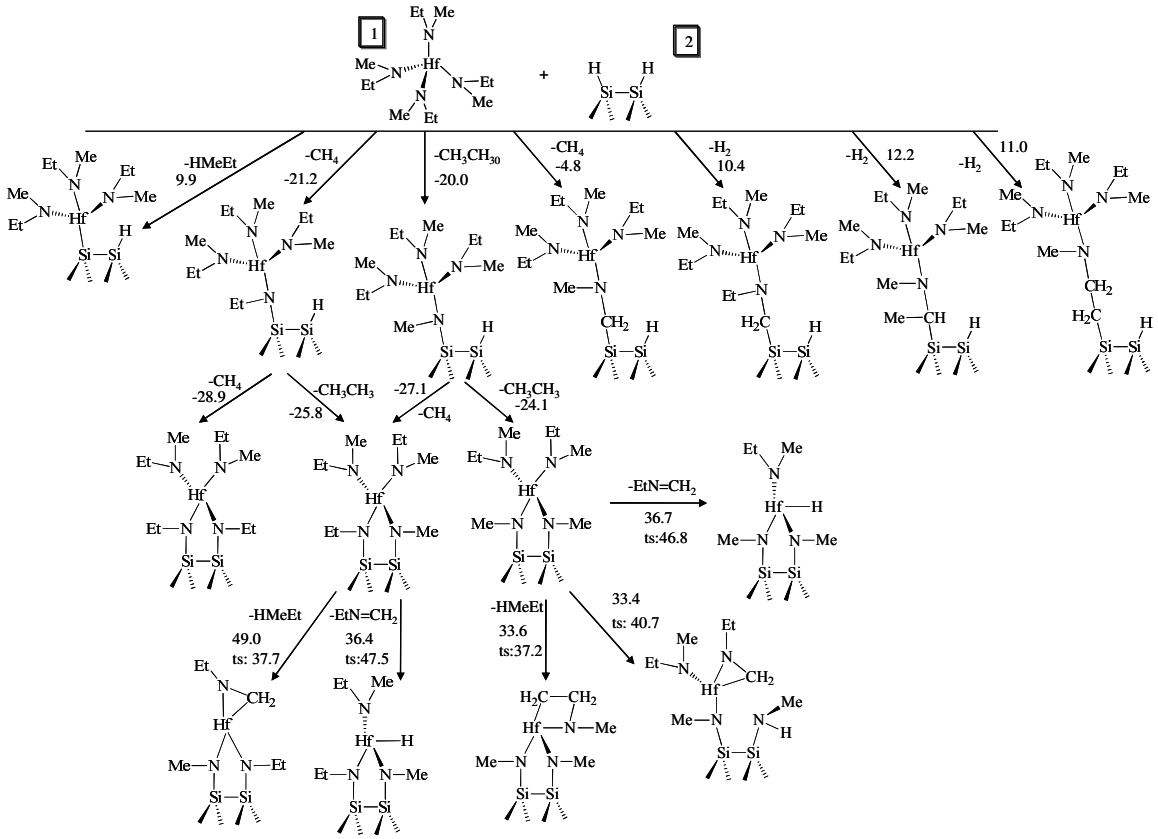
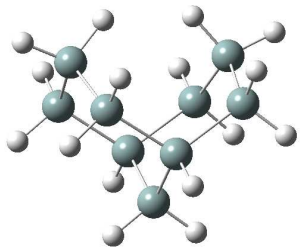
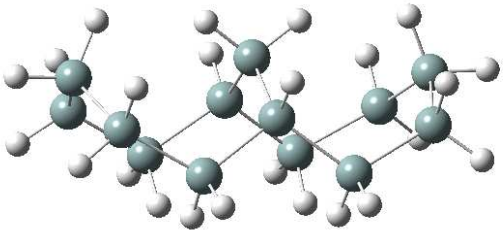


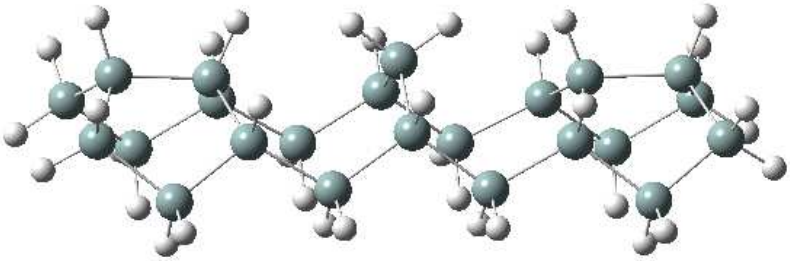
Figure S6. Surface reactions of TEMAH on H-Si(100) calculated at the B3LYP/BS1 level. The overall reaction energies are on the arrows, in kcal/mol. The ts values mean the activation barrier for the transition states. For the insertion reaction by eliminating HMeEt, the reation energy for forming the product complex is 25.9 kcal/mol.



(A)



(B)



(C)

Figure S7. 2×1 and 3×1 H-Si(100) cluster: (A) Si_9H_{16}, (B) $Si_{13}H_{24}$, and (C) $Si_{23}H_{36}$.

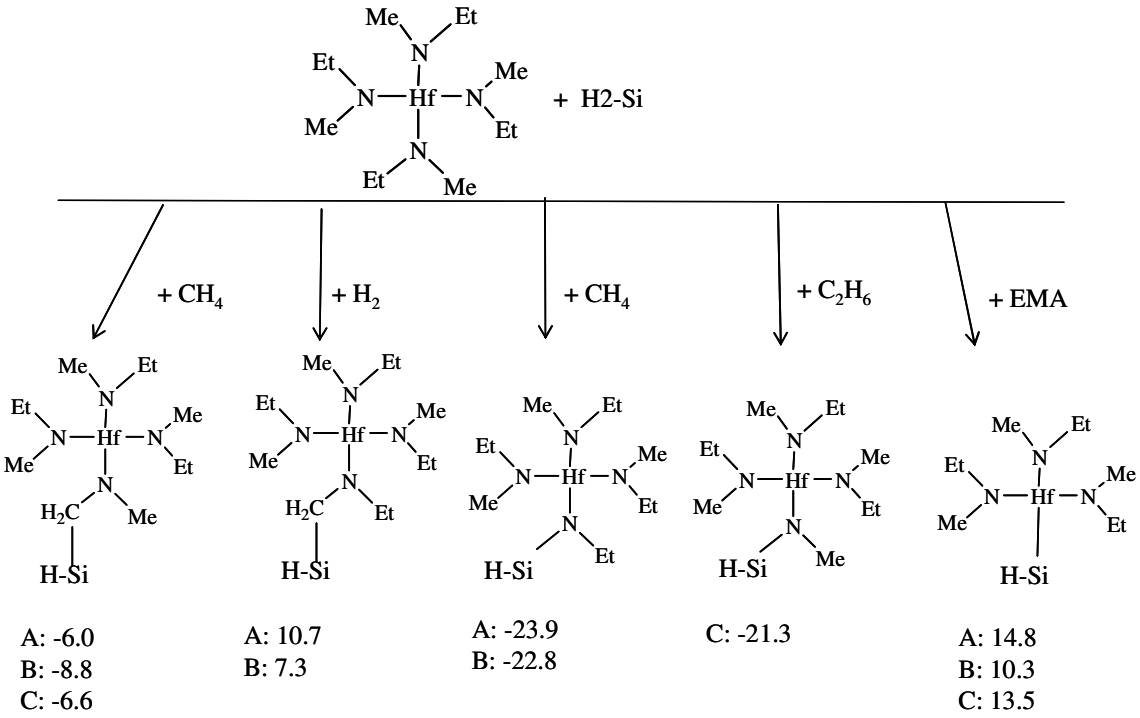


Figure S8: Surface reactions of TEMAH on 2×1 and 3×1 H-Si(100) clusters calculated at the B3LYP/BS1 level. The overall reaction energies are on the arrows, in kcal/mol. (A) Si_9H_{16}, (B) $Si_{13}H_{24}$, and (C) $Si_{23}H_{36}$.

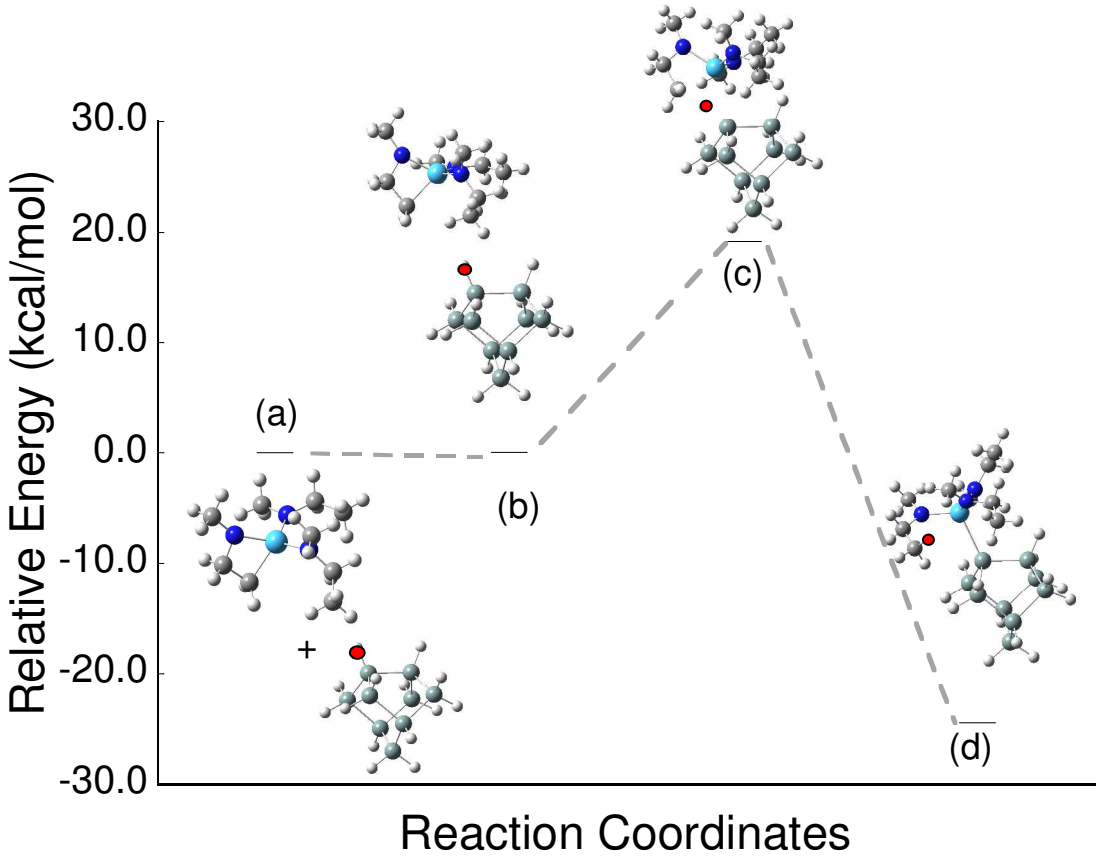


Figure S9. Reaction path of TEI-4 chemisroption onto H-Si(100). The transferred proton is marked in red. The energies are calculated at B3LYP/BS1 level: (a) 0.0, (b) 0.07, (c) 19.1, and (d) -24.4 kcal/mol. The Hf-Si bond length is 2.80 Å.

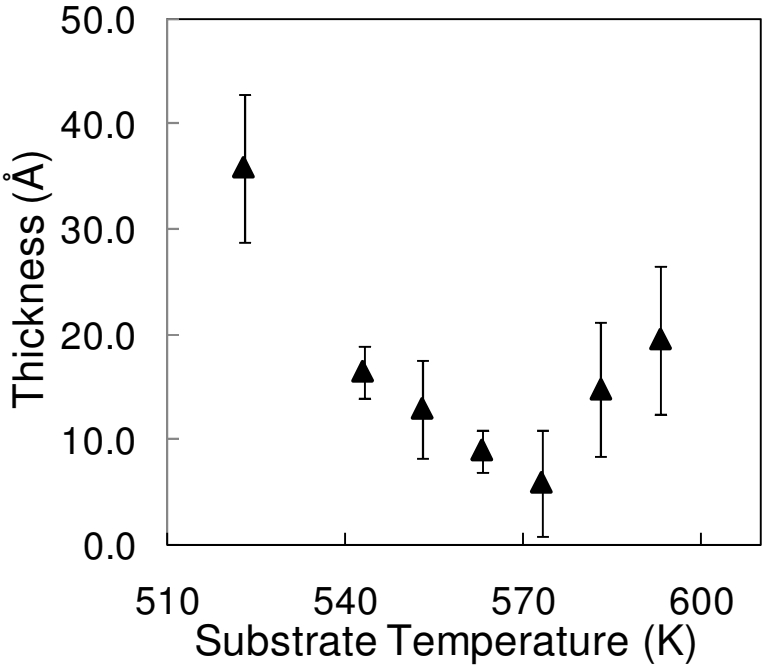


Figure S10. Average thickness of the adlayer as a function of substrate temperature. The error bars are deviations of Hf and N calibrations from the average values.

Structures: Cartesian Coordinates in Å

1: TEMAH

Hf	0.05450100	0.08809600	-0.13662100
N	-0.88172000	-0.60673500	1.55757300
N	-0.46786100	-1.07764800	-1.76549300
N	2.09149000	-0.01590500	0.16724100
N	-0.46771500	2.05106800	-0.55853800
C	-1.75399300	2.74036500	-0.47026600
H	-1.66774900	3.60132100	0.21782600
H	-1.99764400	3.17444700	-1.45768400
C	0.55670300	2.98834200	-1.02037400
H	1.53713700	2.50828100	-1.09046400
H	0.31106100	3.39798400	-2.01533700
H	0.66331300	3.84479000	-0.33233900
C	-0.70625300	0.20550800	2.76084000
H	-0.24068600	-0.37364000	3.57648300
H	-0.04974300	1.06338000	2.55901100
H	-1.65182000	0.61871000	3.14497400
C	-1.66708700	-1.81868000	1.78659100
H	-1.22025300	-2.39429300	2.61748200
H	-1.59219300	-2.45073700	0.89467400
C	2.78115400	-0.38641600	1.40239600
H	2.03187100	-0.71794200	2.13084800
H	3.43336200	-1.25902500	1.21348900
C	2.99976600	0.17217200	-0.96078300
H	3.65345800	-0.70645900	-1.10216900
H	2.43730400	0.30690400	-1.89358900
H	3.65286800	1.05188300	-0.84839400
C	-0.04701500	-2.44576100	-2.07341900
H	-0.94382800	-3.08190000	-2.18549700
H	0.45515300	-2.46431200	-3.05793500
C	-1.34006900	-0.58001900	-2.82961100
H	-2.25350400	-1.19205700	-2.92391600
H	-1.64153300	0.45354200	-2.63886100
H	-0.83361600	-0.60147000	-3.81011000
C	-2.92266800	1.86568600	-0.01813600
H	-3.08502800	1.02340200	-0.70073900
H	-2.75995800	1.46126300	0.98464500
H	-3.84465800	2.45734200	0.00030000
C	0.88226700	-3.08398100	-1.03963700
H	1.82093800	-2.53093300	-0.94353900
H	0.41697000	-3.13277100	-0.04844400
H	1.12137400	-4.10982500	-1.34077300
C	3.62442000	0.73354600	2.03452100
H	3.00190300	1.60613500	2.26226900

H	4.08282400	0.38485000	2.96777200
H	4.43329300	1.06008200	1.37244300
C	-3.15692500	-1.58820500	2.09083100
H	-3.64530400	-1.05938600	1.26572500
H	-3.66574400	-2.54948700	2.23038700
H	-3.30475800	-1.00379100	3.00501600

1a: L3Hf-H

Hf	0.107914	-0.264340	-0.441531
N	-0.200878	1.749210	-0.333339
N	1.662623	-0.888133	0.745402
N	-1.535478	-1.401421	-0.023820
C	-2.891743	-1.257423	0.489846
H	-3.615340	-1.571291	-0.283085
H	-3.033356	-1.955638	1.334045
C	-1.248227	-2.796814	-0.375808
H	-0.225869	-2.908374	-0.769071
H	-1.338699	-3.463584	0.497413
H	-1.925527	-3.167919	-1.159998
C	-1.080877	2.288989	-1.371868
H	-0.556317	3.027365	-1.998999
H	-1.421476	1.489421	-2.045997
H	-1.981019	2.770216	-0.962073
C	0.378973	2.770617	0.536665
H	0.861692	3.548997	-0.080816
H	1.173804	2.303909	1.130724
H	0.524593	-0.659185	-2.216764
C	3.058807	-0.472532	0.590614
H	3.398875	0.034102	1.511347
H	3.693365	-1.369709	0.486840
C	1.522281	-1.822678	1.860385
H	1.838354	-1.363546	2.811665
H	0.481390	-2.138928	1.975906
H	2.139058	-2.724758	1.712314
C	-3.233227	0.156206	0.953514
H	-2.557809	0.487159	1.749334
H	-3.165293	0.876459	0.132609
H	-4.256814	0.184731	1.342610
C	3.305948	0.445432	-0.609038
H	3.030548	-0.042419	-1.550928
H	2.742746	1.382416	-0.530286
H	4.367327	0.708594	-0.666796
C	-0.617087	3.441896	1.495775
H	-1.080921	2.699687	2.154089
H	-0.101081	4.180855	2.120021
H	-1.415016	3.964183	0.957896

1a-ts1: MeN=CHCH3

Hf	-0.167122	-0.094085	-0.151878
N	1.808792	-0.234664	-1.662522
N	-0.812397	-1.638606	1.041580
N	-1.641833	1.322983	-0.079952
N	1.333432	0.743217	1.073457
C	2.794865	0.743609	1.063296
H	3.136196	0.329497	0.112780
H	3.167485	1.784628	1.122328
C	0.829922	1.528167	2.205245
H	-0.260556	1.603214	2.178324
H	1.099942	1.090629	3.179443
H	1.229983	2.558532	2.191661
C	2.074740	1.080232	-2.261345
H	1.401921	1.304779	-3.102623
H	1.974814	1.860105	-1.501813
H	3.107242	1.113895	-2.628845
C	1.308453	-1.133406	-2.449917
H	1.103768	-0.903036	-3.504300
H	-0.701568	-0.728151	-1.907774
C	-1.524313	2.409041	-1.053717
H	-0.706560	2.166985	-1.752672
H	-2.433545	2.447350	-1.679495
C	-2.826614	1.413333	0.758398
H	-3.744115	1.495934	0.149987
H	-2.915884	0.519424	1.382436
H	-2.805662	2.282204	1.435872
C	-1.998037	-2.486697	0.855219
H	-1.683778	-3.545426	0.883263
H	-2.665737	-2.354663	1.725865
C	-0.156195	-2.017984	2.295894
H	0.182227	-3.067811	2.266717
H	0.709964	-1.383835	2.485545
H	-0.847517	-1.927253	3.150969
C	3.459920	-0.067955	2.191358
H	3.191330	0.298417	3.187750
H	3.174570	-1.124210	2.129467
H	4.551727	-0.007235	2.102820
C	-2.806606	-2.253189	-0.421418
H	-3.167336	-1.222603	-0.496655
H	-2.218739	-2.459799	-1.319332
H	-3.679877	-2.915625	-0.420320
C	-1.254262	3.801655	-0.459997
H	-0.336335	3.797580	0.137059
H	-1.144455	4.542709	-1.260907

H	-2.076131	4.132230	0.183281
C	1.239484	-2.583494	-2.075317
H	1.291831	-2.728012	-0.993264
H	0.330555	-3.046612	-2.466049
H	2.102959	-3.090097	-2.530451

1a-ts2: EtN=CH2

Hf	-0.143504	0.111966	-0.370650
N	0.291553	-0.926385	1.398282
N	-2.078378	-0.557229	-0.623796
N	2.309872	0.041369	-0.775718
N	-0.363136	2.134116	-0.162461
C	-0.140048	3.156127	0.852868
H	0.455353	3.977008	0.415309
H	-1.108329	3.606722	1.137215
C	-0.972341	2.710025	-1.365014
H	-1.159252	1.938414	-2.125594
H	-1.938638	3.191273	-1.142975
H	-0.318872	3.470196	-1.824267
C	1.502326	-0.766292	2.201541
H	2.006346	-1.734101	2.377192
H	2.210100	-0.098987	1.707146
H	1.292910	-0.334922	3.192018
C	-0.645467	-1.846345	2.059054
H	-0.109228	-2.769099	2.347823
H	-1.415547	-2.140225	1.342544
C	3.028586	-1.240143	-0.698621
H	2.481953	-1.901119	-0.018387
H	3.053539	-1.729357	-1.684948
C	2.069017	0.483895	-1.970193
H	2.420765	-0.015500	-2.878545
H	0.172042	-0.237957	-2.267555
H	1.652588	1.482119	-2.094502
C	-2.540122	-1.823109	-1.192738
H	-3.187992	-2.333372	-0.455727
H	-3.186064	-1.619790	-2.065905
C	-3.231237	0.255740	-0.240539
H	-3.849460	-0.259967	0.514187
H	-2.915196	1.210530	0.188293
H	-3.885728	0.467506	-1.103900
C	0.565104	2.641943	2.103988
H	-0.001384	1.832949	2.575148
H	1.564062	2.263405	1.865062
H	0.675609	3.452785	2.832188
C	-1.428722	-2.784078	-1.618819
H	-0.817089	-2.352185	-2.415958

H	-0.771766	-3.042433	-0.778942
H	-1.867007	-3.717347	-1.989746
C	4.457881	-1.036685	-0.185554
H	4.456749	-0.559066	0.798746
H	4.969872	-2.001395	-0.099879
H	5.031566	-0.402151	-0.869677
C	-1.347674	-1.275369	3.303750
H	-1.932741	-0.387406	3.039560
H	-2.031219	-2.020837	3.728824
H	-0.638873	-0.994620	4.089574

1b: L2Hfc4

Hf	-0.201004	-0.082752	-0.059932
N	-0.758592	1.911995	-0.039467
N	1.708369	-0.550852	0.532778
N	-1.666848	-1.324485	0.505736
C	-1.931755	-1.795753	-0.902647
H	-1.791044	-2.886240	-0.940328
H	-2.981126	-1.577311	-1.156943
C	-2.538318	-1.892600	1.503440
H	-2.292374	-1.496562	2.494011
H	-3.598445	-1.660833	1.301742
H	-2.448642	-2.991128	1.547468
C	2.810022	-0.274033	-0.390075
H	2.412587	0.298750	-1.244646
H	3.549492	0.387653	0.095498
C	2.125414	-1.152496	1.792522
H	2.894113	-0.540494	2.294791
H	1.271319	-1.233619	2.475186
H	2.535775	-2.166109	1.670536
C	-0.055449	3.171960	0.186360
H	-0.296426	3.873602	-0.631849
H	-0.436145	3.647372	1.108841
C	-2.191133	2.168178	-0.221349
H	-2.377270	2.798859	-1.106275
H	-2.747510	1.234224	-0.356377
H	-2.625576	2.685511	0.650927
C	-0.956680	-1.076779	-1.893187
H	-1.489110	-0.464444	-2.625320
H	-0.310137	-1.783548	-2.419581
C	1.462519	3.037420	0.283990
H	1.756491	2.354885	1.088551
H	1.889467	2.662997	-0.653274
H	1.914185	4.014722	0.485938
C	3.528790	-1.514974	-0.942353
H	2.821787	-2.175843	-1.455181

H	4.306103	-1.218150	-1.656238
H	4.013809	-2.088309	-0.145903

1b-ts

Hf	-0.201004	-0.082752	-0.059932
N	-0.758592	1.911995	-0.039467
N	1.708369	-0.550852	0.532778
N	-1.666848	-1.324485	0.505736
C	-1.931755	-1.795753	-0.902647
H	-1.791044	-2.886240	-0.940328
H	-2.981126	-1.577311	-1.156943
C	-2.538318	-1.892600	1.503440
H	-2.292374	-1.496562	2.494011
H	-3.598445	-1.660833	1.301742
H	-2.448642	-2.991128	1.547468
C	2.810022	-0.274033	-0.390075
H	2.412587	0.298750	-1.244646
H	3.549492	0.387653	0.095498
C	2.125414	-1.152496	1.792522
H	2.894113	-0.540494	2.294791
H	1.271319	-1.233619	2.475186
H	2.535775	-2.166109	1.670536
C	-0.055449	3.171960	0.186360
H	-0.296426	3.873602	-0.631849
H	-0.436145	3.647372	1.108841
C	-2.191133	2.168178	-0.221349
H	-2.377270	2.798859	-1.106275
H	-2.747510	1.234224	-0.356377
H	-2.625576	2.685511	0.650927
C	-0.956680	-1.076779	-1.893187
H	-1.489110	-0.464444	-2.625320
H	-0.310137	-1.783548	-2.419581
C	1.462519	3.037420	0.283990
H	1.756491	2.354885	1.088551
H	1.889467	2.662997	-0.653274
H	1.914185	4.014722	0.485938
C	3.528790	-1.514974	-0.942353
H	2.821787	-2.175843	-1.455181
H	4.306103	-1.218150	-1.656238
H	4.013809	-2.088309	-0.145903

1c: L3Hf-NHMe

Hf	-0.050925	-0.024714	0.350472
N	0.756916	1.776942	-0.207989
N	1.090800	-1.575594	-0.369485
N	-1.929539	-0.248877	-0.465655

N	-0.080923	-0.148814	2.406801
C	-0.334270	-1.304549	3.266073
H	-1.240216	-1.184995	3.879900
H	-0.476124	-2.203445	2.654218
H	0.504837	-1.513246	3.946771
C	0.027522	2.961218	0.244527
H	-0.275961	3.599082	-0.602898
H	-0.893622	2.670731	0.770842
H	0.606878	3.584890	0.942103
C	1.933229	2.084588	-1.018433
H	1.642341	2.746605	-1.854173
H	2.288138	1.151663	-1.470948
C	-2.413284	0.418652	-1.674986
H	-1.565919	0.927329	-2.152129
H	-2.764974	-0.340541	-2.397047
C	-2.917288	-1.139389	0.137423
H	-3.289453	-1.877854	-0.593324
H	-2.474588	-1.699560	0.970001
H	-3.789963	-0.605779	0.543980
C	0.748540	-2.525686	-1.428933
H	0.820865	-3.556407	-1.036018
H	-0.300542	-2.368021	-1.703757
C	2.373781	-1.866571	0.271459
H	3.231710	-1.717273	-0.401731
H	2.526172	-1.213601	1.139406
H	2.414481	-2.908196	0.633676
H	0.104656	0.676385	2.972513
C	1.613290	-2.418128	-2.695716
H	1.537491	-1.415806	-3.132044
H	2.669736	-2.618958	-2.489052
H	1.280084	-3.144931	-3.446312
C	-3.537316	1.444374	-1.449812
H	-3.213847	2.228896	-0.756924
H	-3.815290	1.918167	-2.398919
H	-4.438663	0.979200	-1.037492
C	3.094678	2.735674	-0.249524
H	3.425141	2.088934	0.570916
H	3.946551	2.904687	-0.918963
H	2.812614	3.704773	0.175272

1c-ts

Hf	0.109328	0.050913	-0.075896
N	-0.899090	-0.649506	1.541127
N	1.356721	-1.387439	-0.809527
N	1.166401	1.720043	0.415145
N	-1.426081	0.645856	-1.520038

C	-2.608443	-0.351020	-1.766590
H	-2.566349	-0.659068	-2.818332
H	-2.429773	-1.239321	-1.146296
C	-1.052021	1.343443	-2.773604
H	-0.355140	2.161386	-2.567311
H	-0.588417	0.654669	-3.486560
H	-1.956037	1.773942	-3.227886
C	-1.901223	0.253319	2.116289
H	-1.655351	0.508473	3.159851
H	-1.956091	1.191694	1.547164
H	-2.913128	-0.170337	2.093346
C	-0.760808	-1.917425	2.261215
H	-0.582459	-1.708196	3.329982
H	0.138863	-2.423515	1.891965
C	1.225938	2.422620	1.700623
H	0.731735	1.796967	2.452581
H	2.279655	2.512584	2.015689
C	2.005305	2.324158	-0.620895
H	3.055826	2.393806	-0.295200
H	1.991944	1.716775	-1.536718
H	1.672671	3.332929	-0.903952
C	2.809012	-1.362399	-0.998183
H	3.045706	-1.615684	-2.046190
H	3.162980	-0.337600	-0.837489
C	0.735162	-2.632057	-1.270576
H	1.054675	-3.506426	-0.685687
H	-0.358394	-2.575464	-1.187890
H	0.968352	-2.828473	-2.329152
C	-3.784444	0.495325	-1.344970
H	-4.324041	0.118255	-0.471489
H	-2.293441	1.284069	-1.078632
H	-4.481200	0.751674	-2.146977
C	3.591930	-2.299398	-0.065122
H	3.404137	-2.045557	0.983736
H	3.320680	-3.349272	-0.216042
H	4.667968	-2.207200	-0.253187
C	0.577146	3.815108	1.702716
H	-0.474630	3.755369	1.402658
H	0.623037	4.250571	2.707562
H	1.085108	4.506001	1.022172
C	-1.960427	-2.868406	2.128502
H	-2.145572	-3.120570	1.078693
H	-1.765917	-3.798672	2.674867
H	-2.877419	-2.431828	2.535873

1d: L3Hf-N=CHCH3

Hf	-0.043557	-0.039633	-0.215001
N	0.272138	-0.851033	1.650953
N	1.756989	-0.156601	-1.204992
N	-0.696708	1.869458	0.127373
N	-1.523428	-1.021888	-1.214580
C	-2.439856	-1.627606	-1.833379
H	-2.639829	-1.410036	-2.902534
C	-0.862923	-1.285986	2.462852
H	-0.848337	-0.807097	3.456852
H	-1.807023	-1.009725	1.980199
H	-0.889978	-2.375558	2.620874
C	1.562306	-1.073651	2.303706
H	1.545484	-0.618435	3.310452
H	2.332842	-0.540743	1.734750
C	-0.783804	2.625325	1.376953
H	-0.294666	2.040426	2.163058
H	-0.210859	3.565067	1.276612
C	-1.113924	2.634567	-1.047928
H	-0.546263	3.576221	-1.139404
H	-0.941162	2.058549	-1.966985
H	-2.184011	2.889028	-1.033517
C	2.847152	0.740636	-1.561294
H	3.806789	0.277390	-1.269069
H	2.895565	0.859086	-2.659284
C	1.981343	-1.501939	-1.735321
H	2.919538	-1.938636	-1.354223
H	1.167535	-2.185456	-1.448119
H	2.028564	-1.511770	-2.837163
C	-3.347213	-2.686841	-1.249950
H	-3.248854	-3.620501	-1.819876
H	-3.108593	-2.873777	-0.200793
H	-4.396002	-2.373824	-1.340135
C	2.749566	2.119998	-0.911947
H	1.835039	2.641781	-1.210979
H	2.751763	2.045509	0.181021
H	3.604558	2.736385	-1.210560
C	-2.214271	2.964621	1.827354
H	-2.805526	2.051456	1.958968
H	-2.192215	3.501096	2.783518
H	-2.732245	3.602962	1.104368
C	1.980407	-2.548542	2.433883
H	2.046065	-3.019593	1.446990
H	2.961975	-2.625004	2.917086
H	1.270290	-3.124305	3.037115

1d-ts

Hf	-0.022340	-0.026995	0.054489
N	0.456890	1.908792	-0.562256
N	0.235278	-0.143949	2.118658
N	1.193147	-1.301980	-1.033072
N	-1.890988	-0.536096	-0.313347
C	-3.265612	-0.477703	-0.565582
H	-3.588978	-1.500089	-0.976784
H	-3.855177	-0.475887	0.367102
C	-2.907118	-3.225123	0.019445
H	-2.426682	-3.529927	-0.900314
H	-2.299073	-2.903751	0.851479
H	-3.962984	-3.421737	0.157806
C	0.309060	2.265088	-1.969171
H	1.243852	2.688328	-2.377379
H	0.063242	1.377868	-2.565678
H	-0.491566	3.000509	-2.147173
C	0.959148	3.006788	0.257852
H	1.903259	3.387168	-0.174972
H	1.213321	2.612883	1.249520
C	2.615294	-0.990452	-1.190048
H	2.852130	-0.119556	-0.562894
H	3.225261	-1.825410	-0.798610
C	0.817486	-2.565613	-1.653505
H	1.417650	-3.405728	-1.259827
H	-0.235384	-2.779011	-1.452174
H	0.944510	-2.561340	-2.747848
C	1.070735	-0.871490	3.061196
H	1.595731	-0.154360	3.718947
H	0.428901	-1.472339	3.732418
C	-0.681456	0.755297	2.815568
H	-0.143402	1.498017	3.428831
H	-1.311535	1.309779	2.105461
H	-1.365149	0.204855	3.484206
C	-3.728732	0.697116	-1.437872
H	-3.534738	1.648705	-0.929784
H	-3.191005	0.705835	-2.391304
H	-4.804292	0.630946	-1.646796
C	2.099579	-1.786606	2.401861
H	1.618290	-2.524604	1.752152
H	2.807209	-1.214744	1.792924
H	2.670567	-2.323233	3.167496
C	3.066462	-0.679126	-2.627566
H	2.513282	0.175867	-3.030135
H	4.135764	-0.435755	-2.644790
H	2.912512	-1.531471	-3.297533
C	-0.009443	4.190707	0.431326

H	-0.950959	3.858870	0.883196
H	0.435173	4.952506	1.083114
H	-0.243951	4.669793	-0.524789

1e: L2Hf(Et)NCN(Et)

Hf	0.018350	-0.041674	0.045949
N	1.447969	0.147426	-1.438773
N	0.719097	-1.373933	1.467216
N	-1.884678	-0.036137	-0.659215
N	-0.846823	1.718710	0.560871
C	-0.835297	3.050487	1.118887
H	-1.003146	3.801786	0.325689
H	-1.669010	3.171288	1.833623
C	-2.111433	1.329951	-0.118038
H	-2.946719	1.347816	0.605630
H	-2.351550	2.035205	-0.939936
C	1.220602	1.023360	-2.587384
H	1.318363	0.470424	-3.537514
H	0.209057	1.442072	-2.553911
H	1.921372	1.871609	-2.625747
C	2.734144	-0.549795	-1.502169
H	2.829588	-1.057205	-2.479535
H	2.738725	-1.337514	-0.739295
C	-2.928424	-0.584031	-1.499331
H	-3.190942	0.134217	-2.296936
H	-2.522823	-1.469159	-2.004404
C	0.512670	-2.813981	1.539111
H	1.487350	-3.325628	1.635846
H	-0.060863	-3.076974	2.446285
C	1.453816	-0.868465	2.621225
H	2.446531	-1.340833	2.711955
H	1.616821	0.215342	2.539838
H	0.914216	-1.041989	3.567484
C	0.482092	3.358806	1.829445
H	0.645907	2.666520	2.663118
H	1.327788	3.273851	1.137582
H	0.475663	4.377089	2.232779
C	-0.216815	-3.356874	0.308352
H	-1.218167	-2.918443	0.214603
H	0.345925	-3.147413	-0.610977
H	-0.338939	-4.442863	0.374697
C	-4.210305	-0.981871	-0.748306
H	-4.681360	-0.117366	-0.268588
H	-4.940921	-1.417216	-1.440641
H	-3.988055	-1.719752	0.030331
C	3.967291	0.344120	-1.287170

H	3.921596	0.835897	-0.308721
H	4.884841	-0.255467	-1.327040
H	4.048574	1.122500	-2.052953

1e-ts

Hf	0.054970	-0.016817	0.056767
N	1.735779	-0.386546	-1.106254
N	-1.565172	-0.881199	-0.631793
N	-0.632249	1.951804	-0.209322
N	0.120403	-0.418770	2.113393
C	1.227934	-0.233111	3.046139
H	0.895231	0.398510	3.890995
H	1.510860	-1.203731	3.495118
C	-1.026802	-0.973844	2.830191
H	-1.866871	-1.134316	2.151249
H	-0.783895	-1.942747	3.302895
H	-1.361720	-0.300756	3.640286
C	2.911960	0.475736	-1.112825
H	3.135930	0.835085	-2.132554
H	2.749188	1.362650	-0.487914
H	3.821093	-0.016332	-0.732186
C	1.833889	-1.488725	-2.063841
H	2.077921	-1.089766	-3.065373
H	0.845820	-1.958273	-2.159637
C	-0.282970	2.841440	-1.317072
H	0.504463	2.364842	-1.912278
H	-1.151816	2.957797	-1.986000
C	-1.896531	2.169958	0.373004
H	-2.287369	3.193395	0.284271
H	-2.652475	1.451976	-0.171897
H	-1.952909	1.831719	1.413926
C	-3.620481	0.306888	-0.971168
H	-3.283799	0.151865	-1.987080
H	-3.937072	-0.565436	-0.418125
C	-2.089515	-2.093743	-1.178366
H	-1.349211	-2.574771	-1.844140
H	-2.941811	-1.874153	-1.854861
C	2.471014	0.400247	2.423889
H	2.889413	-0.231239	1.633182
H	2.245527	1.387885	2.001361
H	3.248045	0.541708	3.182955
C	0.198742	4.226967	-0.858769
H	1.094711	4.137108	-0.235924
H	0.440959	4.853653	-1.725044
H	-0.568324	4.744230	-0.272649
C	2.857486	-2.577117	-1.698118

H	2.620378	-3.018555	-0.723624
H	2.850559	-3.376224	-2.449266
H	3.876412	-2.178794	-1.650111
H	-4.276557	1.166361	-0.842187
C	-2.567760	-3.123224	-0.136682
H	-3.354825	-2.702613	0.499237
H	-2.966392	-4.019826	-0.628387
H	-1.742407	-3.426281	0.516076

1f: L3Hf-N=CH2

Hf	-0.015996	0.037703	0.341406
N	-0.944449	-1.439618	-0.726071
N	-1.049172	1.792327	-0.020741
N	1.953168	0.187680	-0.232674
N	-0.161384	-0.388566	2.329379
C	-0.148531	-0.782984	3.524626
H	0.421299	-1.668468	3.860247
H	-0.710500	-0.267599	4.324180
C	-0.373296	-2.780011	-0.590926
H	-0.080347	-3.194549	-1.569991
H	0.530389	-2.755460	0.033719
H	-1.064485	-3.491950	-0.116438
C	-2.110702	-1.385516	-1.606376
H	-1.867055	-1.869662	-2.568804
H	-2.321879	-0.333400	-1.826532
C	2.671295	-0.481271	-1.313382
H	1.946162	-1.051315	-1.906894
H	3.102238	0.275422	-1.994637
C	2.755290	1.178159	0.482446
H	3.193031	1.919600	-0.208253
H	2.133817	1.734558	1.198981
H	3.577832	0.731854	1.060958
C	-0.922902	2.738097	-1.129430
H	-1.928734	2.943234	-1.537702
H	-0.549767	3.709429	-0.755430
C	-2.032963	2.284536	0.945917
H	-3.026917	2.401732	0.481827
H	-2.132010	1.594012	1.788331
H	-1.745695	3.269595	1.353274
C	-0.022403	2.263427	-2.270522
H	1.006159	2.102462	-1.933881
H	-0.388498	1.324105	-2.702354
H	-0.005715	3.012000	-3.070252
C	3.792089	-1.429775	-0.856245
H	3.394231	-2.213567	-0.202069
H	4.260839	-1.910381	-1.723275

H	4.577599	-0.899013	-0.308395
C	-3.380440	-2.031870	-1.028347
H	-3.666303	-1.544348	-0.089997
H	-4.212737	-1.932784	-1.735418
H	-3.243036	-3.099671	-0.828231

1f-ts

Hf	-0.206774	-0.317890	-0.050062
N	0.303387	1.709526	-0.320579
N	-0.758025	-0.710161	1.927239
N	1.322955	-1.428730	-0.546599
N	-1.760684	-0.881706	-1.314896
C	-3.045253	-0.225864	-1.542318
H	-3.202064	-0.083264	-2.627724
H	-3.864376	-0.893624	-1.212894
C	-1.702285	-2.123286	-2.086831
H	-0.743901	-2.625268	-1.936493
H	-2.506161	-2.821521	-1.792750
H	-1.822394	-1.932700	-3.168499
C	0.582070	2.168608	-1.676037
H	1.586948	2.623766	-1.757439
H	0.545937	1.330307	-2.382475
H	-0.139347	2.920022	-2.036538
C	0.394029	2.775705	0.674451
H	1.363578	3.298349	0.574336
H	0.388280	2.321057	1.672662
C	3.948084	0.349140	-0.126648
H	4.692663	0.130164	0.632625
H	2.925120	0.527370	0.183366
C	2.441653	-2.172516	-0.842841
H	3.291384	-1.991242	-0.119871
H	2.258731	-3.253927	-0.976526
H	2.940353	-1.839704	-1.804358
C	0.097363	-0.750735	3.108162
H	-0.284692	-0.047275	3.871371
H	0.033800	-1.753229	3.570321
C	-2.125683	-1.075678	2.286678
H	-2.556885	-0.372384	3.020625
H	-2.774444	-1.087000	1.406373
H	-2.167006	-2.081289	2.739857
C	-3.203361	1.128216	-0.850100
H	-3.079059	1.048268	0.236902
H	-2.472477	1.853165	-1.219266
H	-4.205820	1.529890	-1.035030
C	1.567726	-0.434157	2.833322
H	1.986839	-1.127431	2.095450

H	1.697487	0.588400	2.459450
H	2.150611	-0.521228	3.756793
C	4.291406	0.376849	-1.532777
H	3.676700	1.086222	-2.102204
H	5.356999	0.512794	-1.736904
H	4.005109	-0.622544	-1.981670
C	-0.730070	3.826757	0.623042
H	-1.706809	3.360297	0.786095
H	-0.575903	4.582120	1.403225
H	-0.759010	4.348753	-0.339149

1g: L2Hf(Me)NCN(Et)

Hf	-0.050586	-0.133199	-0.018528
N	-1.292347	1.233273	-0.955553
N	0.724082	0.501991	1.747513
N	1.911839	0.279030	-0.295694
N	-0.757344	-2.048953	-0.360083
C	-1.766228	-2.756541	0.417134
H	-2.573863	-3.109162	-0.249525
H	-1.333287	-3.663005	0.877617
C	-0.195497	-2.882817	-1.416268
H	0.553001	-2.328292	-1.997970
H	0.307796	-3.778608	-1.014818
H	-0.971834	-3.225662	-2.121183
C	-2.453001	0.918991	-1.784948
H	-2.361088	1.370267	-2.788221
H	-2.546176	-0.163941	-1.914491
H	-3.399530	1.280678	-1.352665
C	-1.033783	2.673904	-0.864263
H	-0.986779	3.103743	-1.881076
H	-0.039434	2.822770	-0.424155
C	3.033526	0.544416	-1.171672
H	2.680034	0.461493	-2.206741
H	3.376098	1.586993	-1.044401
C	2.064532	0.675149	1.129606
H	2.399513	1.730018	1.200778
H	2.804993	0.041998	1.652622
C	0.659280	0.797854	3.156268
H	-0.357709	0.632754	3.526077
H	1.338532	0.159393	3.746859
H	0.925698	1.846651	3.372700
C	-2.372361	-1.877335	1.513910
H	-1.610798	-1.563313	2.239755
H	-2.847390	-0.982549	1.090363
H	-3.143059	-2.421239	2.069590
C	4.230499	-0.400530	-0.974441

H	3.931278	-1.441459	-1.138208
H	5.033830	-0.155225	-1.679633
H	4.640970	-0.323145	0.038117
C	-2.057239	3.464186	-0.032603
H	-2.091215	3.085022	0.994871
H	-1.783574	4.525706	0.002008
H	-3.065774	3.397391	-0.453849

1g-ts

Hf	0.212315	-0.116076	0.068283
N	1.791332	0.022406	-1.279741
N	-0.981706	-1.611771	-0.325771
N	-1.153208	1.453534	-0.202307
N	0.650662	-0.301708	2.112985
C	1.623663	0.447133	2.899501
H	1.118078	0.924481	3.760291
H	2.369473	-0.242378	3.338568
C	-0.003940	-1.294979	2.960996
H	-0.733036	-1.872653	2.386932
H	0.723644	-2.002709	3.398655
H	-0.534045	-0.821629	3.807773
C	2.572483	1.234897	-1.492476
H	2.556407	1.537881	-2.554409
H	2.161900	2.071680	-0.913937
H	3.629780	1.135404	-1.198158
C	2.200908	-1.075563	-2.155823
H	2.213020	-0.727357	-3.205097
H	1.438295	-1.864076	-2.107977
C	-1.245631	2.331904	-1.365735
H	-0.399715	2.122306	-2.031320
H	-2.156542	2.094132	-1.942013
C	-2.365460	1.273166	0.526029
H	-3.068339	2.115617	0.453536
H	-2.884139	0.338398	0.128091
H	-2.183192	1.050378	1.584378
C	-3.502702	-1.384353	-0.470557
H	-3.076595	-1.577739	-1.444150
H	-3.261547	-2.088796	0.312221
C	-1.095701	-2.995687	-0.615871
H	-0.434386	-3.325438	-1.436494
H	-0.906965	-3.645232	0.257962
H	-2.121781	-3.265697	-0.960958
C	2.360132	1.523090	2.103480
H	2.946952	1.080923	1.291488
H	1.658072	2.250669	1.675752
H	3.050540	2.076201	2.749424

C	-4.847927	-0.726231	-0.418411
H	-5.118158	-0.379177	0.583446
H	-4.946321	0.104009	-1.123479
H	-5.599607	-1.483280	-0.707363
C	-1.245315	3.828012	-1.010624
H	-0.317337	4.100709	-0.497217
H	-1.332040	4.438988	-1.917090
H	-2.081556	4.083929	-0.351138
C	3.567689	-1.698643	-1.822477
H	3.571964	-2.095233	-0.800924
H	3.791506	-2.521520	-2.512421
H	4.380203	-0.968997	-1.905111

1h: L2Hfc3

Hf	-0.019841	-0.141427	0.062169
N	-1.252366	1.398347	-0.565750
N	1.901434	0.285753	0.021008
N	-0.489126	-2.123076	-0.308554
C	-1.694737	-2.716767	0.261579
H	-2.398716	-3.025931	-0.532188
H	-1.432302	-3.636810	0.812745
C	0.295059	-3.095757	-1.060081
H	1.212451	-2.637870	-1.443416
H	0.589607	-3.952762	-0.431189
H	-0.266183	-3.498065	-1.920746
C	-2.503671	1.281295	-1.307646
H	-2.450386	1.820365	-2.268558
H	-2.717989	0.231152	-1.537861
H	-3.369296	1.679424	-0.756149
C	-0.832134	2.790059	-0.360857
H	-0.789690	3.308995	-1.334820
H	0.195027	2.786537	0.028749
C	3.089199	0.961546	-0.459118
H	3.003978	1.076349	-1.548262
H	3.139067	1.980193	-0.033873
C	1.576307	0.279615	1.489681
H	1.729764	1.268550	1.949637
H	2.089717	-0.494763	2.071690
C	-2.405084	-1.758982	1.224971
H	-1.744738	-1.474112	2.058298
H	-2.759328	-0.848921	0.722277
H	-3.287178	-2.229110	1.670936
C	4.392181	0.221191	-0.128071
H	4.392510	-0.778685	-0.575414
H	5.258830	0.773738	-0.510828
H	4.510882	0.109019	0.954759

C	-1.715571	3.599265	0.601981
H	-1.752831	3.120594	1.586901
H	-1.312048	4.610962	0.727460
H	-2.741471	3.697939	0.232142

1h-ts

Hf	-0.084050	0.048403	-0.119169
N	1.189379	0.242151	1.472259
N	0.002823	1.696962	-1.236193
N	-2.023162	-0.214131	0.538249
N	0.465357	-1.775346	-1.367155
C	1.565026	-2.713547	-1.117754
H	1.343111	-3.349989	-0.243138
H	1.645556	-3.398115	-1.977713
C	-0.684177	-2.410119	-2.013368
H	-1.407596	-1.648036	-2.329701
H	-0.379480	-2.966779	-2.913704
H	-1.211541	-3.106142	-1.344447
C	1.273859	-0.907940	2.370571
H	0.947670	-0.653353	3.392953
H	0.625231	-1.725334	2.020952
H	2.289555	-1.325947	2.438788
C	1.955886	1.401865	1.931765
H	1.679031	1.632381	2.975900
H	1.656449	2.264839	1.328240
C	-2.447833	-0.488612	1.911428
H	-1.574797	-0.411281	2.570754
H	-3.150095	0.297305	2.243182
C	-3.147582	0.009480	-0.367834
H	-3.816666	0.802108	0.008905
H	-2.790487	0.331199	-1.353470
H	-3.758505	-0.893243	-0.522730
C	-0.334775	3.065419	-1.561051
H	0.581320	3.618954	-1.831312
H	-0.978007	3.089452	-2.459097
C	0.653880	0.847981	-2.247453
H	1.690627	1.150362	-2.469341
H	0.726278	-0.641034	-1.957126
H	0.084000	0.814188	-3.192212
C	2.913980	-2.018408	-0.919156
H	3.198701	-1.453447	-1.813282
H	2.891461	-1.323401	-0.074032
H	3.693882	-2.762467	-0.725207
C	-1.042313	3.775102	-0.405690
H	-1.964695	3.250994	-0.132421
H	-0.400873	3.815506	0.482007

H	-1.301962	4.802852	-0.682867
C	-3.105943	-1.862619	2.122656
H	-2.419522	-2.669536	1.841606
H	-3.381005	-1.996605	3.175789
H	-4.017645	-1.973025	1.526743
C	3.482132	1.244268	1.843182
H	3.793697	1.066645	0.808313
H	3.976573	2.156853	2.196470
H	3.847703	0.414414	2.457460

CH3CH3

C	-0.766308	-0.000002	-0.000002
H	-1.165252	0.676317	-0.764264
H	-1.165324	-1.000017	-0.203526
C	0.766308	0.000002	0.000001
H	1.165243	-0.676302	0.764280
H	1.165248	-0.323793	-0.967811
H	1.165315	1.000024	0.203510
H	-1.165234	0.323773	0.967819

MeN=CHCH3

N	-0.684726	0.721260	-0.000052
C	0.588234	0.666524	0.000018
H	1.095827	1.638049	0.000105
C	-1.511782	-0.474096	-0.000001
H	-0.979496	-1.434847	-0.001374
H	-2.165200	-0.440786	0.879374
H	-2.167255	-0.439478	-0.877781
C	1.527152	-0.518008	-0.000016
H	1.026077	-1.487056	0.000647
H	2.180375	-0.465907	-0.879919
H	2.181134	-0.465309	0.879313

EtN=CH2

N	0.694771	-0.245038	-0.459695
C	-0.468610	0.570487	-0.130166
H	-0.688889	1.187459	-1.010764
H	-0.266792	1.253424	0.713994
C	1.747123	-0.095474	0.233428
H	1.827694	0.621036	1.066545
H	2.628186	-0.697802	0.006650
C	-1.680038	-0.314545	0.176707
H	-2.567224	0.302008	0.356584
H	-1.886135	-0.986747	-0.661783
H	-1.501092	-0.926915	1.066830

HNEtMe

N	-0.658421	0.529366	-0.396810
C	0.635571	0.611617	0.286387
H	1.088978	1.571476	0.012867
H	0.520567	0.612969	1.388499
C	-1.549854	-0.510082	0.111616
H	-1.705723	-0.466629	1.206253
H	-2.524314	-0.423567	-0.378639
H	-1.151227	-1.500692	-0.128945
C	1.584024	-0.519900	-0.118026
H	1.734540	-0.522514	-1.202465
H	2.556950	-0.394342	0.370312
H	1.195609	-1.501525	0.173534
H	-1.124882	1.429450	-0.343606

2: H-Si(100)

Si	0.00032400	-0.00094300	2.48118800
H	0.00045600	-1.20353500	3.36315300
H	0.00042500	1.20060700	3.36456100
Si	1.96347400	-0.00043600	1.15135800
H	3.17592500	-0.00070300	2.02024000
Si	-1.96317600	-0.00022300	1.15185500
H	-3.17542400	-0.00018800	2.02101400
Si	1.88766400	1.80158600	-0.37592900
H	3.13456200	1.83265000	-1.19226300
H	1.72104300	3.13323700	0.27038900
Si	-1.88730800	1.80181300	-0.37542600
Si	-0.00003700	1.19839100	-1.67475400
H	-3.13428400	1.83283300	-1.19165400
H	-1.72057200	3.13353700	0.27070400
Si	-1.88794300	-1.80109800	-0.37683300
H	-1.72217800	-3.13347500	0.26818500
H	-3.13474700	-1.83060400	-1.19338000
Si	1.88731400	-1.80169200	-0.37684300
Si	-0.00023400	-1.19738900	-1.67536700
H	3.13416500	-1.83264000	-1.19324800
H	1.72041600	-3.13361000	0.26885100
H	-0.00036200	1.79115500	-3.04254200
H	-0.00052100	-1.78936500	-3.04350900

2a: L3Hf-Si

Hf	2.02574400	-0.19534000	-0.08846300
N	2.13944600	-1.54250200	1.43333300
N	2.83638700	1.61421400	0.36194400
N	2.82855700	-0.88555400	-1.83541600
C	2.87336700	-0.07830300	-3.06375700

H	3.88579200	0.34164900	-3.19680800
H	2.70531900	-0.74098100	-3.92772800
C	3.55280600	-2.14392500	-2.00418900
H	3.54491900	-2.72899500	-1.07949500
H	3.10551800	-2.76044200	-2.79973600
H	4.60660100	-1.96881900	-2.27432700
C	2.24652600	2.39365900	1.45921500
H	3.00718100	2.56321900	2.23968800
C	3.99808500	2.25218400	-0.25041100
H	4.76563900	2.48180700	0.50611600
H	4.45077200	1.58581200	-0.99096500
H	3.74400800	3.19251100	-0.76040100
C	2.67962700	-1.66773700	2.78490700
H	1.86865200	-1.96365800	3.47159000
H	3.40626700	-2.49852400	2.79975300
C	1.54961500	-2.81737700	0.99958100
H	0.70686400	-3.11202400	1.64232600
H	1.15251400	-2.75414100	-0.02466800
H	2.29032400	-3.63270900	1.01286300
C	1.83264000	1.04742800	-3.12271000
H	2.00494700	1.66285900	-4.01223200
H	1.86422000	1.72458700	-2.25658100
C	3.35257000	-0.40705400	3.31823100
H	4.14069800	-0.05919300	2.64187300
H	2.63363000	0.40526400	3.45469300
H	3.80673300	-0.61473300	4.29286000
C	1.63392300	3.73954300	1.04605700
H	0.86126600	3.60027100	0.28375500
H	1.17453100	4.22273300	1.91583300
H	2.38863300	4.42644000	0.65033100
H	-1.13028400	3.20542200	-1.07022700
Si	-1.80753900	1.90808700	-1.36986600
Si	-3.97843600	1.95713800	-0.43590200
H	-1.82191900	1.76954800	-2.85593400
Si	-0.74501300	0.05365500	-0.32452800
Si	-5.17010300	0.01783900	-1.09540800
H	-4.76403400	3.18529400	-0.76151200
Si	-3.39987300	1.77859800	1.84532700
Si	-1.76419200	-1.71172400	-1.55863300
Si	-1.92813200	-0.07460200	1.76661600
H	0.82039300	0.63840300	-3.19179900
H	-5.46257300	0.08480600	-2.55735100
H	-6.48348800	-0.03286100	-0.38816400
Si	-3.92357500	-1.94302600	-0.63118600
H	-2.70628600	3.02241800	2.29299600
H	-4.56167200	1.55846500	2.75389900

H	-1.03123500	-3.00568000	-1.40344300
H	-1.78765900	-1.41461000	-3.02141000
Si	-3.33122500	-1.97938300	1.65395700
H	-1.02074400	-0.11744000	2.95336300
H	-4.67126400	-3.15739100	-1.07586800
H	-2.58622500	-3.23630500	1.96218100
H	-4.49115700	-1.90245600	2.58778700
H	1.45712100	1.78819000	1.93026500

2b: L3Hf-EtN-Si

Hf	-2.117369	-0.018462	0.154913
N	-0.541555	-0.454453	-1.159154
N	-3.881822	-0.700489	-0.683874
N	-2.319875	2.009043	0.411373
N	-1.948149	-0.912112	2.008874
C	-1.558496	-2.275281	2.375555
H	-0.670446	-2.237278	3.031364
H	-2.360874	-2.724763	2.988253
C	-2.217368	-0.143317	3.226014
H	-2.503468	0.885890	2.995339
H	-3.031465	-0.598135	3.814900
H	-1.327915	-0.096951	3.876662
C	-0.829397	-0.915228	-2.548069
H	0.005339	-0.654218	-3.216338
H	-1.694596	-0.369057	-2.943048
C	-1.506857	3.099818	-0.126849
H	-0.676254	2.665841	-0.695348
H	-2.105536	3.681130	-0.852465
C	-3.543398	2.477320	1.061850
H	-4.100831	3.175888	0.414234
H	-4.214039	1.636141	1.278535
H	-3.351711	2.993303	2.014723
C	-4.589695	-0.186865	-1.861708
H	-4.517117	-0.924607	-2.681975
H	-5.665826	-0.111086	-1.627052
C	-4.597192	-1.867268	-0.164065
H	-4.645708	-2.681639	-0.907747
H	-4.116516	-2.258296	0.735741
H	-5.636708	-1.611261	0.101766
C	-1.259816	-3.203141	1.198807
H	-2.131776	-3.335668	0.549791
H	-0.435534	-2.831123	0.585244
H	-0.975869	-4.193297	1.570916
C	-4.123997	1.176749	-2.375546
H	-4.299518	1.965020	-1.639378
H	-3.058876	1.190163	-2.631506

H	-4.678169	1.431592	-3.285614
C	-0.940497	4.065303	0.926168
H	-0.342046	3.526742	1.668368
H	-0.299181	4.813013	0.445792
H	-1.733904	4.603870	1.454678
C	-1.109776	-2.417492	-2.661643
H	-1.994080	-2.687936	-2.075791
H	-1.294784	-2.692103	-3.707448
H	-0.266434	-3.013557	-2.299107
H	5.026385	2.929881	-1.551190
Si	4.234737	1.809870	-0.962993
Si	5.619925	-0.073982	-0.590061
Si	2.336246	1.218910	-2.243669
Si	3.160066	2.372279	1.061213
H	6.727428	0.299000	0.336806
H	6.240377	-0.512499	-1.873637
Si	4.366725	-1.862644	0.323981
Si	1.176032	-0.301098	-0.809342
H	1.536036	2.450922	-2.510243
H	2.693589	0.623306	-3.563614
H	4.091416	2.569121	2.208217
H	2.369811	3.624085	0.893215
Si	1.769519	0.480619	1.393165
H	5.237189	-3.056034	0.537237
Si	2.489395	-2.290166	-1.046214
Si	3.226419	-1.166837	2.272970
H	0.617333	0.771214	2.290163
H	1.788563	-3.504165	-0.535727
H	2.856948	-2.555694	-2.467599
H	2.473842	-2.318350	2.848573
H	4.107315	-0.613955	3.340234

2c: L3Hf-MeN-Si

Hf	-2.147188	-0.082666	0.040311
N	-0.537728	-0.387804	-1.267822
N	-3.905495	-0.489983	-0.966593
N	-2.292612	1.846512	0.739018
N	-2.110095	-1.360693	1.656225
C	-1.806973	-2.793319	1.683915
H	-0.925305	-2.972319	2.324809
H	-2.643494	-3.325202	2.172047
C	-2.382583	-0.883847	3.012838
H	-2.605435	0.186319	3.018002
H	-3.240735	-1.413615	3.459383
H	-1.516962	-1.043436	3.677513
C	-0.778733	-0.876327	-2.646333

H	-0.392352	-0.180909	-3.406513
H	-1.849421	-1.006069	-2.831891
C	-1.378577	2.969675	0.531337
H	-0.491835	2.603155	-0.000155
H	-1.850109	3.711854	-0.139671
C	-3.566584	2.251998	1.332920
H	-4.028718	3.081763	0.769775
H	-4.280491	1.419344	1.324669
H	-3.463852	2.578958	2.378478
C	-4.446550	0.274787	-2.094084
H	-4.504273	-0.378601	-2.984343
H	-5.488691	0.564613	-1.870818
C	-4.807869	-1.592738	-0.639774
H	-4.918909	-2.292591	-1.486256
H	-4.442055	-2.156401	0.221847
H	-5.818240	-1.224338	-0.392572
C	-1.558846	-3.422131	0.312191
H	-2.430776	-3.322146	-0.344165
H	-0.699771	-2.970035	-0.190820
H	-1.354420	-4.492107	0.425535
C	-3.661977	1.538030	-2.457295
H	-3.662373	2.261782	-1.637155
H	-2.619719	1.318348	-2.716032
H	-4.117420	2.016450	-3.331020
C	-0.927400	3.687489	1.812868
H	-0.455778	2.985939	2.508986
H	-0.200554	4.470336	1.569124
H	-1.765942	4.166921	2.327844
H	5.043590	3.030674	-1.188836
Si	4.225748	1.861359	-0.752078
Si	5.586576	-0.067848	-0.566870
Si	2.349970	1.446371	-2.132186
Si	3.112029	2.205296	1.301032
H	6.678005	0.189042	0.416911
H	6.230434	-0.361874	-1.879839
Si	4.308729	-1.942171	0.111328
Si	1.173229	-0.224176	-0.895507
H	1.563407	2.707945	-2.267996
H	2.727820	1.001321	-3.504440
H	4.020023	2.283738	2.480195
H	2.320303	3.466086	1.246842
Si	1.719395	0.289482	1.393025
H	5.172035	-3.156044	0.201859
Si	2.467735	-2.188451	-1.347744
Si	3.142542	-1.462744	2.108229
H	0.533704	0.470917	2.276749

H	1.732702	-3.439962	-1.001933
H	2.879790	-2.290438	-2.777552
H	2.368219	-2.660361	2.543060
H	4.013396	-1.041224	3.241530
H	-0.303566	-1.853434	-2.822071

2d: L3Hf-MeNCH2-Si

Hf	2.658008	-0.126408	-0.210885
N	2.452118	0.403161	1.776321
N	3.622333	1.316194	-1.330790
N	0.829628	-0.617627	-1.059923
N	3.768543	-1.864608	-0.349183
C	5.014368	-2.240029	0.321025
H	4.868519	-3.189704	0.866983
H	5.781872	-2.454309	-0.445389
C	3.366180	-2.935739	-1.263871
H	2.427501	-2.690631	-1.768103
H	4.132231	-3.112489	-2.038139
H	3.220748	-3.890054	-0.729102
C	1.972703	-0.586443	2.739470
H	1.037970	-0.262375	3.227522
H	1.772948	-1.545296	2.245253
H	2.704103	-0.796735	3.534918
C	2.685571	1.716208	2.381985
H	1.761750	2.063837	2.878414
H	2.895980	2.434118	1.580944
C	-0.170594	-1.414363	-0.364366
H	0.199956	-1.692582	0.631052
C	0.480797	-0.366232	-2.451864
H	-0.416005	0.268461	-2.551973
H	1.301367	0.140624	-2.969171
H	0.272225	-1.305254	-2.993099
C	3.167833	2.677413	-1.624374
H	3.846644	3.405988	-1.144997
H	3.253258	2.860227	-2.710197
C	4.946613	1.098193	-1.915987
H	5.689139	1.807262	-1.511808
H	5.301589	0.084210	-1.714605
H	4.928290	1.235753	-3.010205
C	5.568787	-1.196411	1.290280
H	5.764766	-0.241133	0.788840
H	4.880350	-1.007783	2.117802
H	6.517595	-1.548401	1.709837
C	1.730249	2.975302	-1.196616
H	1.012268	2.337057	-1.719819
H	1.580663	2.842462	-0.119668

H	1.479885	4.016053	-1.428027
C	3.843616	1.781937	3.392069
H	4.788592	1.490092	2.922562
H	3.951237	2.805343	3.770372
H	3.675873	1.130348	4.255501
H	-6.345392	-2.272397	1.859183
Si	-5.364431	-1.426798	1.117733
Si	-5.732383	0.868815	1.578104
Si	-5.371259	-1.781463	-1.217148
Si	-3.107916	-1.960615	1.561366
H	-5.622959	1.104478	3.047060
H	-7.116363	1.246109	1.169076
Si	-4.166483	2.237041	0.440117
Si	-3.480079	-0.506065	-1.856804
H	-5.185841	-3.231925	-1.510930
H	-6.617696	-1.329700	-1.897681
H	-2.687347	-1.665144	2.961160
H	-2.883171	-3.417650	1.322587
Si	-1.931160	-0.639796	-0.025805
H	-4.417721	3.675135	0.751186
Si	-4.219715	1.744093	-1.871248
Si	-1.963810	1.529773	0.929457
H	-2.904613	-0.944378	-3.161414
H	-3.273052	2.635247	-2.602326
H	-5.565072	1.895991	-2.493556
H	-0.997679	2.461611	0.284313
H	-1.665031	1.499667	2.389602
H	-0.349721	-2.369396	-0.892525

2e: L3Hf-EtNCH2-Si

Hf	2.680743	0.075629	0.013729
N	0.957167	-1.073318	-0.156726
N	3.992022	-0.799821	1.349007
N	2.262165	2.003261	0.610707
N	3.684778	0.242605	-1.789380
C	3.969369	-0.760799	-2.814974
H	3.567383	-0.420826	-3.786636
H	5.063794	-0.829721	-2.955784
C	4.270574	1.523474	-2.191968
H	4.083552	2.297962	-1.444247
H	5.362044	1.439357	-2.329979
H	3.848697	1.878577	-3.147890
C	0.022278	-0.712852	-1.219339
H	0.335832	0.239886	-1.671321
H	0.027404	-1.438946	-2.051227
C	0.613766	-2.293578	0.573441

H	-0.411861	-2.208011	0.975542
H	1.273237	-2.367648	1.445042
C	0.969636	2.685412	0.563083
H	0.204949	1.959316	0.261003
H	0.687049	3.016385	1.578912
C	3.309680	2.814597	1.228105
H	3.000007	3.183014	2.221737
H	4.222638	2.223824	1.368454
H	3.582927	3.693784	0.623897
C	3.825159	-0.915918	2.799898
H	3.843128	-1.983763	3.083939
H	4.694968	-0.458859	3.305248
C	5.272769	-1.381867	0.948772
H	5.326299	-2.455024	1.200198
H	5.431409	-1.275434	-0.127447
H	6.116543	-0.887409	1.459889
C	3.424117	-2.156565	-2.519864
H	3.819582	-2.555436	-1.578358
H	2.332694	-2.158182	-2.457343
H	3.716960	-2.847274	-3.318107
C	2.550618	-0.275910	3.354882
H	2.525467	0.801859	3.169199
H	1.644942	-0.714982	2.921041
H	2.499370	-0.431988	4.437784
C	0.903864	3.891551	-0.388292
H	1.145971	3.593450	-1.414314
H	-0.104262	4.321863	-0.384320
H	1.599841	4.683096	-0.092193
C	0.720497	-3.603466	-0.223525
H	1.749674	-3.778141	-0.550883
H	0.413042	-4.448405	0.403641
H	0.076363	-3.604066	-1.108781
H	-6.074933	-2.926007	0.576015
Si	-5.115145	-1.801745	0.370508
Si	-6.232303	0.080651	-0.537519
Si	-3.271676	-2.366770	-0.995256
Si	-3.952806	-1.169028	2.327111
H	-7.311763	0.520483	0.393169
H	-6.881507	-0.299978	-1.825366
Si	-4.725157	1.871498	-0.908565
Si	-1.865002	-0.465032	-0.755299
H	-2.640990	-3.617712	-0.484506
H	-3.644701	-2.602068	-2.419875
H	-4.814619	-0.546098	3.371008
H	-3.288248	-2.360418	2.929560
Si	-2.377327	0.360809	1.438622

H	-5.440213	3.040178	-1.500286
Si	-2.899038	1.110440	-2.202886
Si	-3.585898	2.369907	1.101191
H	-1.181608	0.531980	2.310510
H	-1.985419	2.253317	-2.498949
H	-3.303299	0.508196	-3.505237
H	-2.681722	3.538019	0.897913
H	-4.490050	2.682824	2.243625

2f: L3Hf-MeN-MeCH-Si

Hf	-2.607762	-0.193373	0.036533
N	-2.394486	1.855096	0.004970
N	-3.459699	-0.830841	1.804374
N	-0.811033	-1.201994	-0.309667
N	-3.918983	-0.821005	-1.431816
C	-4.965883	-0.183593	-2.228815
H	-4.661571	-0.151235	-3.291255
H	-5.867376	-0.821108	-2.199262
C	-3.797546	-2.230253	-1.815636
H	-3.022449	-2.740114	-1.233147
H	-4.744725	-2.771753	-1.653473
H	-3.532158	-2.345763	-2.880584
C	-1.798194	2.507204	-1.158683
H	-0.848980	3.009445	-0.906800
H	-1.584650	1.777049	-1.949830
H	-2.461256	3.261044	-1.608785
C	-2.675750	2.793221	1.095838
H	-1.750587	3.335423	1.362673
H	-2.964705	2.215608	1.980977
C	0.130705	-0.808823	-1.357061
H	-0.157632	0.197097	-1.694252
C	-0.500872	-2.473076	0.338486
H	0.461445	-2.440627	0.876134
H	-1.272829	-2.719856	1.074593
H	-0.446855	-3.315544	-0.368515
C	-2.887549	-0.744891	3.150112
H	-3.532721	-0.108316	3.782293
H	-2.906719	-1.745487	3.618031
C	-4.797407	-1.422951	1.873534
H	-5.471068	-0.819372	2.505095
H	-5.241997	-1.494989	0.878155
H	-4.766150	-2.435830	2.309761
C	-5.355800	1.220873	-1.775117
H	-5.717774	1.214804	-0.740877
H	-4.515040	1.916548	-1.831356
H	-6.160023	1.605932	-2.411890

C	-1.456244	-0.209921	3.201972
H	-0.761511	-0.855126	2.656494
H	-1.378184	0.800539	2.786317
H	-1.114271	-0.158805	4.241114
C	0.097622	-1.723559	-2.603737
H	-0.926303	-1.793930	-2.988448
H	0.734600	-1.327194	-3.402811
H	0.444290	-2.738338	-2.383229
C	-3.785676	3.818747	0.811879
H	-4.731128	3.317241	0.581685
H	-3.939616	4.454146	1.691877
H	-3.536160	4.476885	-0.026560
H	6.065408	-2.610346	1.342755
Si	5.130709	-1.560062	0.841317
Si	6.335209	0.137076	-0.292108
Si	3.796982	-0.587937	2.531576
Si	3.429564	-2.400528	-0.570630
H	7.111161	-0.468042	-1.413246
H	7.316570	0.764695	0.639679
Si	4.875156	1.797385	-1.143010
Si	2.320855	0.727706	1.228695
H	3.068726	-1.653752	3.278859
H	4.564381	0.221770	3.519660
H	3.951638	-2.862816	-1.888635
H	2.771810	-3.568796	0.082571
Si	1.995254	-0.515008	-0.795784
H	5.645018	2.838629	-1.885221
Si	3.553057	2.655180	0.615234
Si	3.167029	0.775497	-2.415044
H	1.054761	1.060175	1.937378
H	2.662442	3.735859	0.101167
H	4.339344	3.211996	1.752280
H	2.291204	1.832365	-3.004956
H	3.682057	-0.054247	-3.541927

2g: L3Hf-MeN-CH2CH2-Si

Hf	2.567237	-0.113091	0.199955
N	2.832310	0.948407	-1.529331
N	4.388112	-0.974792	0.651997
N	1.152322	-1.616361	-0.127922
N	2.130666	1.062038	1.847269
C	2.104244	2.490386	2.151344
H	1.088409	2.780908	2.475140
H	2.759331	2.681870	3.020892
C	1.763999	0.303898	3.044626
H	1.791901	-0.777409	2.864217

H	2.458543	0.507372	3.877359
H	0.746914	0.545454	3.393666
C	1.652663	1.601862	-2.089853
H	1.414704	1.219115	-3.096481
H	0.770415	1.420088	-1.460796
H	1.759611	2.693984	-2.165587
C	4.023318	1.079849	-2.370428
H	3.790918	0.725254	-3.390863
H	4.795356	0.412990	-1.972295
C	0.526511	-1.935054	-1.410116
H	0.641069	-1.077829	-2.082981
H	1.073973	-2.772706	-1.885647
C	1.033157	-2.712180	0.831590
H	1.282704	-3.683524	0.368617
H	1.728061	-2.578380	1.668578
H	0.025099	-2.802781	1.264449
C	5.059414	-2.096598	-0.007896
H	6.055064	-1.763637	-0.352801
H	5.253682	-2.896504	0.729483
C	5.224450	-0.481474	1.748828
H	6.200110	-0.123834	1.378447
H	4.737462	0.347104	2.269528
H	5.431044	-1.274413	2.488238
C	2.536318	3.400834	1.005634
H	3.549360	3.163643	0.665654
H	1.863931	3.316950	0.147190
H	2.524924	4.444610	1.338260
C	4.305577	-2.694564	-1.196267
H	3.344216	-3.118829	-0.893192
H	4.117639	-1.946967	-1.975508
H	4.900976	-3.496489	-1.646123
C	-0.961830	-2.364455	-1.380562
H	-1.231005	-2.687852	-2.396320
H	-1.081319	-3.256640	-0.753560
C	4.603950	2.500120	-2.460749
H	4.890692	2.867316	-1.469811
H	5.496504	2.500770	-3.097486
H	3.891580	3.210392	-2.893038
H	-4.019487	3.592705	-1.457167
Si	-3.879227	2.219208	-0.890597
Si	-6.012140	1.291819	-0.435664
Si	-2.536246	2.125861	1.051887
Si	-2.655169	0.751084	-2.281896
H	-6.818956	1.265514	-1.689885
H	-6.735149	2.156515	0.541423
Si	-5.811407	-0.903008	0.432051

Si	-2.344391	-0.214752	1.351290
H	-1.215009	2.761622	0.783598
H	-3.140624	2.805503	2.232398
H	-3.382573	0.376787	-3.528574
H	-1.380462	1.405320	-2.693188
Si	-2.339073	-1.130427	-0.865327
H	-7.159249	-1.489124	0.689149
Si	-4.401699	-0.874635	2.325550
Si	-4.458104	-2.203371	-1.001727
H	-1.177379	-0.609497	2.184402
H	-4.318660	-2.242955	2.914035
H	-4.843538	0.060340	3.398815
H	-4.385853	-3.599540	-0.476056
H	-4.966087	-2.276348	-2.401891

3a: L2Hf-EtN-Si

Hf	-1.704780	-0.006033	-0.045256
N	-3.404336	0.287017	1.064548
N	-2.378808	-0.636207	-1.880435
N	-0.505522	-1.395289	0.929882
N	-0.545881	1.711380	-0.310743
C	-0.850017	3.112065	-0.655728
H	-0.046263	3.771052	-0.293126
H	-0.870048	3.235863	-1.751307
C	-3.261626	0.859421	2.404015
H	-3.672049	0.185274	3.174418
H	-2.204133	1.024085	2.646742
H	-3.765558	1.831906	2.508795
C	-4.785162	-0.075329	0.738746
H	-5.184611	-0.735531	1.529692
H	-4.773224	-0.662995	-0.185621
C	-0.902950	-2.590681	1.697386
H	-1.936774	-2.849683	1.437539
H	-0.292922	-3.456593	1.395628
C	-2.661076	-1.946305	-2.462023
H	-3.675649	-1.931110	-2.898016
H	-1.973766	-2.135322	-3.305578
C	-2.578201	0.415285	-2.881274
H	-3.614143	0.418342	-3.257549
H	-2.375787	1.408256	-2.463791
H	-1.908143	0.285905	-3.746875
C	-2.173453	3.610368	-0.071949
H	-3.023365	3.018066	-0.427891
H	-2.161455	3.553853	1.021291
H	-2.344293	4.653555	-0.361466
C	-2.567399	-3.103328	-1.470756

H	-1.557498	-3.199035	-1.061484
H	-3.268714	-2.970715	-0.638156
H	-2.819999	-4.045823	-1.967909
C	-0.817116	-2.415484	3.218220
H	-1.442855	-1.578727	3.544806
H	-1.164077	-3.324051	3.725336
H	0.207762	-2.218970	3.547883
C	-5.745946	1.110524	0.554747
H	-5.404038	1.767370	-0.252585
H	-6.748164	0.747467	0.297741
H	-5.837760	1.711630	1.465202
H	4.541722	-1.256595	-3.134634
Si	3.797417	-0.751183	-1.943002
Si	5.335120	0.001239	-0.304382
Si	2.354051	-2.356138	-0.970012
Si	2.255568	0.975662	-2.437220
H	6.188653	1.084884	-0.872430
H	6.239855	-1.118634	0.086733
Si	4.213996	0.812847	1.618039
Si	1.184982	-1.017755	0.618653
H	1.433642	-2.900221	-2.011123
H	3.091604	-3.505007	-0.368785
H	2.918665	2.222583	-2.917863
H	1.322104	0.515695	-3.507195
Si	1.144281	1.210816	-0.339564
H	5.202225	1.273172	2.637379
Si	2.699413	-0.802591	2.445777
Si	2.653341	2.476894	1.000733
H	2.033877	-0.255156	3.663547
H	3.340522	-2.096216	2.820022
H	1.990700	3.022680	2.221243
H	3.263244	3.618501	0.260468

3b: L2Hf-MeEtN-Si

Hf	1.860221	0.095920	-0.194415
N	0.720087	-0.358169	1.495284
N	3.447931	1.344772	0.231421
N	0.581093	0.975600	-1.565428
N	2.740495	-1.524678	-1.103711
C	3.361810	-2.714577	-0.526560
H	2.791634	-3.615387	-0.815238
H	4.367830	-2.841175	-0.964826
C	2.757534	-1.600350	-2.565797
H	2.295750	-0.715810	-3.015041
H	3.788468	-1.674121	-2.949914
H	2.203973	-2.480261	-2.933059

C	1.127629	-0.446349	2.909884
H	0.765131	0.439299	3.456797
H	2.223388	-0.406235	2.959855
C	0.888398	1.784136	-2.750712
H	0.374923	2.756701	-2.727734
H	1.964133	1.986940	-2.812727
H	0.594602	1.277713	-3.682441
C	3.358139	2.672596	0.845407
H	3.980179	2.697115	1.757910
H	3.798509	3.420154	0.161774
C	4.844018	1.032220	-0.074579
H	5.464839	1.024782	0.837777
H	4.925993	0.052335	-0.550942
H	5.283279	1.779699	-0.756966
C	3.486557	-2.665227	0.994817
H	4.085422	-1.805164	1.318826
H	2.502557	-2.602786	1.468103
H	3.979917	-3.569755	1.365683
C	1.936464	3.107878	1.202789
H	1.291352	3.138966	0.317391
H	1.480512	2.435562	1.937663
H	1.949244	4.112825	1.637678
C	0.644490	-1.702278	3.645262
H	0.988460	-2.614751	3.147958
H	1.024106	-1.708016	4.673791
H	-0.449465	-1.740055	3.698838
H	-4.483730	-3.108307	-1.350635
Si	-3.707052	-1.930742	-0.861609
Si	-5.201152	-0.271368	-0.066521
Si	-2.269462	-0.994314	-2.493519
Si	-2.141056	-2.451250	0.834461
H	-6.035089	-0.836771	1.033742
H	-6.128416	0.137143	-1.161559
Si	-4.041811	1.637319	0.725638
Si	-1.088319	0.592806	-1.168007
H	-1.366069	-2.054480	-3.028986
H	-3.005296	-0.395321	-3.644332
H	-2.785796	-2.915666	2.097269
H	-1.232809	-3.536469	0.361588
Si	-0.987237	-0.378655	1.054972
H	-5.010133	2.662517	1.214390
Si	-2.585111	2.434677	-0.955965
Si	-2.441288	1.002935	2.344616
H	-1.891415	3.666207	-0.477712
H	-3.280602	2.768095	-2.232121
H	-1.745513	2.219351	2.857790

H	-3.028420	0.288150	3.514310

3c: L2Hf-MeN-Si

Hf	1.814811	-0.127520	-0.031301
N	0.611992	0.047674	1.652483
N	2.713230	1.624119	-0.607355
N	0.564539	-0.770448	-1.560169
N	3.268181	-1.543493	0.301304
C	4.720965	-1.657415	0.212049
H	5.135039	-1.857849	1.216929
H	4.975170	-2.544078	-0.395910
C	2.692090	-2.804449	0.785022
H	1.599645	-2.738991	0.873570
H	2.913851	-3.640711	0.102229
H	3.080441	-3.073928	1.781012
C	0.965353	0.051690	3.077542
H	0.440141	-0.740725	3.630495
H	2.040225	-0.116386	3.210845
H	0.722629	1.009390	3.561218
C	0.906071	-1.381563	-2.850212
H	0.676986	-0.715464	-3.695752
H	1.976721	-1.614499	-2.896326
H	0.363987	-2.324211	-3.015129
C	3.190682	2.777544	0.151438
H	4.251019	2.957865	-0.100735
H	2.647302	3.684292	-0.168049
C	2.918591	1.839741	-2.040792
H	3.984975	1.993804	-2.273856
H	2.571922	0.982296	-2.628196
H	2.367378	2.723725	-2.400805
C	5.424679	-0.440304	-0.382214
H	5.090020	-0.246945	-1.406738
H	5.237889	0.462560	0.206498
H	6.505986	-0.614951	-0.407297
C	3.059477	2.624454	1.665231
H	2.013288	2.518317	1.966621
H	3.614096	1.750329	2.028479
H	3.468843	3.505801	2.170035
H	-4.464294	3.304579	-0.808778
Si	-3.712985	2.050969	-0.503503
Si	-5.245601	0.304113	-0.039628
Si	-2.194483	2.266489	1.301558
Si	-2.244641	1.374264	-2.234584
H	-6.140888	0.099371	-1.215342
H	-6.109179	0.690154	1.113992
Si	-4.130969	-1.725761	0.460141

Si	-1.080217	0.164885	1.182171
H	-1.268611	3.407352	1.041650
H	-2.874631	2.518179	2.604920
H	-2.962378	0.988201	-3.483801
H	-1.316885	2.494626	-2.568093
Si	-1.114823	-0.432620	-1.166254
H	-5.125646	-2.799807	0.751318
Si	-2.576785	-1.378402	2.207288
Si	-2.634649	-2.264946	-1.288678
H	-1.902336	-2.667675	2.539498
H	-3.198514	-0.851567	3.455914
H	-1.961404	-3.563064	-0.990696
H	-3.300100	-2.387587	-2.617386

4a: c3-Hf-MeEtN-Si

Hf	-2.053177	-0.124996	-0.149852
N	-0.960803	1.583967	0.281049
N	-4.024111	-0.182327	-0.103125
N	-0.883697	-1.810226	-0.413357
C	-1.383143	2.945724	0.658415
H	-0.852714	3.268431	1.567900
H	-2.448812	2.917462	0.920276
C	-1.191576	-3.218116	-0.693353
H	-0.845919	-3.880436	0.113539
H	-2.272799	-3.359611	-0.798607
H	-0.722796	-3.558063	-1.627532
C	-5.402199	-0.338039	0.302147
H	-5.968884	0.579734	0.070929
H	-5.876835	-1.145566	-0.280946
C	-3.698566	0.107139	-1.543535
H	-4.063763	1.083152	-1.891728
H	-4.012924	-0.688724	-2.233782
C	-5.520819	-0.648971	1.795788
H	-4.996423	-1.579758	2.041648
H	-5.087865	0.159135	2.396697
H	-6.570512	-0.763715	2.087726
C	-1.175643	3.986982	-0.446877
H	-1.708224	3.693482	-1.357105
H	-1.550781	4.965561	-0.124668
H	-0.115441	4.102584	-0.696716
H	4.652713	0.517612	-2.919923
Si	3.719891	0.287256	-1.778072
Si	4.954026	-0.065720	0.213706
Si	2.224851	-1.510796	-2.126589
Si	2.152042	2.029514	-1.465886
H	5.818435	1.120046	0.480793

H	5.852008	-1.244201	0.042151
Si	3.523600	-0.430707	2.066948
Si	0.794355	-1.293064	-0.236280
H	1.480624	-1.307104	-3.402950
H	2.900069	-2.838640	-2.187780
H	2.772635	3.323673	-1.060789
H	1.402982	2.253735	-2.735725
Si	0.742393	1.120879	0.224726
H	4.331023	-0.647382	3.303144
Si	2.022920	-2.195376	1.593010
Si	1.971231	1.343153	2.252390
H	1.139588	-2.427315	2.773694
H	2.700389	-3.482103	1.264380
H	1.097829	1.116921	3.441438
H	2.612828	2.680631	2.400487

4a-ts

Hf	1.861430	0.107855	-0.220501
N	0.744773	0.003212	1.523616
N	3.355810	1.410228	-0.014018
N	0.579765	0.692620	-1.730239
N	2.634285	-1.931763	-0.832510
C	2.723566	-3.097388	0.053931
H	1.720986	-3.508303	0.257574
H	3.285407	-3.892503	-0.462055
C	2.415789	-2.296912	-2.233587
H	2.510776	-1.412419	-2.874646
H	3.162577	-3.032774	-2.570466
H	1.416993	-2.723475	-2.407273
C	1.158576	0.214485	2.924509
H	0.725504	1.154106	3.302197
H	2.246862	0.353494	2.946686
C	0.886117	1.302312	-3.030161
H	0.389908	2.275746	-3.154004
H	1.964057	1.473426	-3.131960
H	0.573438	0.659756	-3.866349
C	3.928904	2.707396	0.272898
H	4.711038	2.604441	1.045197
H	4.438890	3.095758	-0.626067
C	4.218141	0.322833	-0.500649
H	4.993672	0.031792	0.227677
H	3.577261	-1.013760	-0.720377
H	4.703617	0.555804	-1.463819
C	3.426520	-2.781449	1.376024
H	4.459805	-2.459994	1.209739
H	2.906813	-1.993062	1.931250

H	3.445526	-3.669949	2.015572
C	2.873164	3.709870	0.739378
H	2.113236	3.865952	-0.034367
H	2.368478	3.352544	1.643877
H	3.331685	4.678748	0.965458
C	0.777716	-0.924931	3.877143
H	1.203205	-1.877972	3.546834
H	1.147324	-0.714645	4.887624
H	-0.309466	-1.047507	3.942497
H	-4.482906	-3.261011	-0.663676
Si	-3.703397	-2.010056	-0.426796
Si	-5.188238	-0.221282	0.033157
Si	-2.282210	-1.419127	-2.226801
Si	-2.113276	-2.189687	1.318090
H	-6.016371	-0.554584	1.228293
H	-6.120345	-0.037025	-1.116872
Si	-4.020183	1.802776	0.425469
Si	-1.089235	0.400375	-1.258036
H	-1.378216	-2.564592	-2.542228
H	-3.025649	-1.068422	-3.471016
H	-2.731947	-2.408735	2.657480
H	-1.204144	-3.340780	1.041956
Si	-0.970021	-0.111906	1.112175
H	-4.983868	2.904741	0.715631
Si	-2.578984	2.255877	-1.391272
Si	-2.409065	1.491095	2.126329
H	-1.873524	3.550635	-1.164744
H	-3.286386	2.338858	-2.701094
H	-1.706285	2.779733	2.391792
H	-2.989801	1.010134	3.412474

4b: H-Hf-MeEtN-Si

H	-5.638415	1.203047	0.416969
H	-5.646799	-1.200383	0.365386
H	-4.587563	0.065071	-2.876823
H	-4.039380	-0.071341	3.435721
H	-1.387582	-1.774188	-3.174062
H	-2.750246	-3.098724	-1.681800
H	-0.843916	-1.904223	3.087276
H	-2.429781	3.093774	1.947185
H	-0.832221	1.756295	3.166588
H	-1.388341	1.917699	-3.094966
H	-2.748525	3.172040	-1.541238
Hf	2.249469	0.006380	-0.368767
N	4.069592	-0.023359	0.542137
N	1.082786	1.678936	-0.143380

N	1.077208	-1.667973	-0.219443
C	4.743674	-1.224166	1.024078
C	4.881376	1.170633	0.754314
C	1.442951	3.101440	-0.099804
C	1.447206	-3.087377	-0.283464
H	4.948563	-1.166126	2.105142
H	4.127532	-2.114931	0.857036
H	5.704518	-1.380538	0.508548
H	5.078845	1.343646	1.824411
H	5.852304	1.091106	0.240716
H	4.379020	2.063781	0.363890
H	1.177642	3.560812	0.862901
H	2.522210	3.236070	-0.241413
H	0.943522	3.671365	-0.895446
H	1.188599	-3.618968	0.643249
H	0.947734	-3.599670	-1.117309
H	2.526811	-3.203890	-0.440648
H	2.726052	0.054778	-2.151577
H	-2.444043	-3.173462	1.800478
Si	-0.621834	-1.210872	-0.072581
Si	-0.617638	1.214253	-0.021543
Si	-2.087123	1.857283	-1.779825
Si	-1.756604	1.764485	1.995314
Si	-3.270882	-0.044521	2.156752
Si	-1.765000	-1.851194	1.914585
Si	-3.604216	0.040842	-1.754307
Si	-2.088715	-1.774379	-1.858744
Si	-4.762749	-0.000099	0.314282

4b-ts

Hf	-1.811448	-0.090325	-0.181352
N	-0.516857	-1.660180	0.283147
N	-3.440871	-1.796001	-0.671877
N	-0.452648	1.396129	-0.768721
N	-2.948979	0.558611	1.407945
C	-3.584410	1.828772	1.747294
H	-4.631369	1.632458	2.041054
H	-3.099328	2.262331	2.639692
C	-3.067311	-0.376380	2.529706
H	-2.626167	-1.349545	2.288627
H	-2.553897	0.002010	3.428149
H	-4.122647	-0.546228	2.801313
C	-0.840103	-3.026293	0.729964
H	-0.524306	-3.200077	1.769888
H	-1.915901	-3.206620	0.658164
H	-0.339521	-3.781757	0.105650

C	-0.730224	2.554736	-1.648132
H	-0.294605	2.374785	-2.644018
H	-1.811234	2.623011	-1.806527
C	-4.855667	-1.773913	-0.242433
H	-5.307458	-2.717484	-0.579084
H	-4.853543	-1.804506	0.849427
C	-3.174810	-1.589829	-1.930895
H	-3.932382	-1.421047	-2.701010
H	-2.564243	0.261517	-1.943167
H	-2.178087	-1.829758	-2.301490
C	-3.568168	2.860610	0.623558
H	-2.546972	3.156750	0.374615
H	-4.048685	2.476373	-0.284238
H	-4.110789	3.760553	0.931810
C	-5.715068	-0.595040	-0.716019
H	-5.311110	0.354739	-0.357306
H	-5.797311	-0.543668	-1.806241
H	-6.729028	-0.706462	-0.317051
H	5.175891	-1.096763	-2.749434
Si	4.202485	-0.724545	-1.680104
Si	5.367827	-0.116368	0.291758
Si	2.630779	-2.422064	-1.184429
Si	2.722573	1.013780	-2.302431
H	6.278215	1.028097	-0.005137
H	6.222900	-1.256776	0.733217
Si	3.881559	0.486798	2.037083
Si	1.194443	-1.240215	0.302747
H	1.922776	-2.825191	-2.435864
H	3.248060	-3.646236	-0.596996
H	3.412387	2.315402	-2.535850
H	2.027417	0.635407	-3.568138
Si	1.238379	1.027651	-0.435798
H	4.663687	0.855020	3.254565
Si	2.332284	-1.267070	2.392994
Si	2.424605	2.189113	1.274081
H	1.428162	-0.914111	3.527446
H	2.985206	-2.567667	2.720133
H	1.526201	2.609732	2.389223
H	3.149492	3.401940	0.794456
C	-0.212669	3.897526	-1.118278
H	0.881609	3.918249	-1.061820
H	-0.520946	4.711517	-1.785228
H	-0.601241	4.107255	-0.116150

4c: c4-Hf-MeN-Si

Hf	2.159824	0.000065	0.045923

N	1.001798	-1.702411	-0.129180
N	4.073795	0.000283	-0.549857
N	1.001717	1.702575	-0.128473
C	1.354916	-3.119910	-0.277816
H	0.989493	-3.720098	0.567698
H	2.443127	-3.241931	-0.320893
C	1.354848	3.120139	-0.276486
H	0.989601	3.719931	0.569385
H	2.443054	3.242148	-0.319709
H	0.938522	3.553360	-1.197534
C	4.608912	-0.000565	0.862318
H	5.239299	-0.892071	0.999676
H	5.239980	0.890335	1.000442
C	5.089449	0.000288	-1.575259
H	5.739626	-0.887627	-1.504679
H	4.628721	0.001033	-2.568040
H	5.740507	0.887482	-1.503768
C	3.414543	-0.000555	1.867423
H	3.399832	0.890130	2.500517
H	3.399515	-0.891433	2.500205
H	-4.509175	0.000514	-3.110263
Si	-3.597526	0.000373	-1.928776
Si	-4.863913	-0.000237	0.073452
Si	-2.067152	1.801862	-1.913153
Si	-2.067272	-1.801249	-1.913624
H	-5.747097	-1.202062	0.098250
H	-5.747526	1.201254	0.098999
Si	-3.471335	-0.000481	1.990478
Si	-0.693705	1.221437	-0.056358
H	-1.291703	1.813149	-3.187927
H	-2.718928	3.133656	-1.758529
H	-2.719160	-3.133009	-1.759170
H	-1.291821	-1.812420	-3.188395
Si	-0.693652	-1.221353	-0.056799
H	-4.314335	-0.000678	3.222258
Si	-1.960774	1.816719	1.871149
Si	-1.960278	-1.817237	1.870792
H	-1.113287	1.851205	3.098033
H	-2.645654	3.135274	1.744966
H	-1.112570	-1.851306	3.097538
H	-2.644772	-3.136013	1.744873
H	0.938754	-3.552669	-1.199153

4c-ts

Hf	1.861390	-0.201437	-0.139729
N	0.706848	-0.186787	1.579904

N	2.623694	1.905132	-0.311201
N	0.555597	-0.583872	-1.703552
N	3.179901	-1.694501	0.300620
C	4.405097	-1.403696	-0.446158
H	5.233423	-1.178342	0.249494
H	4.724742	-2.285320	-1.031879
C	3.213976	-2.891187	1.115688
H	2.267091	-3.022096	1.649042
H	3.385012	-3.793427	0.505080
H	4.023559	-2.849604	1.864794
C	1.090764	-0.289934	2.994555
H	0.499620	-1.051867	3.523265
H	2.143730	-0.577339	3.086795
H	0.955614	0.662064	3.528351
C	0.791453	-1.171001	-3.031476
H	0.432223	-0.511499	-3.835069
H	1.860320	-1.337444	-3.198945
H	0.288071	-2.141627	-3.146396
C	3.125870	2.688667	0.826296
H	3.666564	3.568644	0.442266
H	2.280459	3.075504	1.417170
C	2.063998	2.758647	-1.365740
H	2.800087	3.505755	-1.701245
H	1.776538	2.152723	-2.230789
H	1.170371	3.300387	-1.024558
C	4.104047	-0.181045	-1.341869
H	3.744151	-0.501173	-2.330833
H	3.466620	1.062211	-0.817099
H	5.017483	0.395187	-1.534814
C	4.067129	1.890404	1.731416
H	3.583021	0.997566	2.142233
H	4.963473	1.569297	1.191236
H	4.385607	2.506573	2.578435
H	-4.418149	3.381008	-0.311792
Si	-3.668656	2.096825	-0.177871
Si	-5.197002	0.314298	0.142266
Si	-2.067182	2.109690	1.568462
Si	-2.275646	1.612482	-2.031904
H	-6.141767	0.259406	-1.010802
H	-6.006997	0.563620	1.369941
Si	-4.080977	-1.764983	0.351415
Si	-0.999991	0.015167	1.186450
H	-1.127937	3.252283	1.365889
H	-2.676265	2.253746	2.921946
H	-3.042595	1.360847	-3.285811
H	-1.358697	2.762819	-2.280448

Si	-1.111774	-0.294590	-1.207161
H	-5.073533	-2.863002	0.541757
Si	-2.482538	-1.618848	2.084766
Si	-2.637712	-2.102207	-1.490015
H	-1.805254	-2.935551	2.266656
H	-3.069572	-1.216978	3.395072
H	-1.962856	-3.426228	-1.360093
H	-3.339839	-2.069292	-2.804708

4d: c3-Hf-MeN-Si-Si-NHMe

Hf	1.958815	-0.144890	0.132266
N	0.542539	-1.360431	-0.871142
N	3.565632	-1.258854	0.488965
N	0.379243	0.765785	1.691033
N	2.547389	1.580773	-0.871914
C	3.679182	2.478255	-0.654097
H	4.382581	2.403075	-1.503809
H	3.323789	3.525280	-0.655183
C	1.833386	1.959907	-2.090875
H	1.013338	1.264846	-2.303293
H	1.401807	2.973207	-2.017457
H	2.498640	1.953729	-2.971403
C	0.906353	-2.519768	-1.710744
H	0.676315	-2.349825	-2.773684
H	1.978353	-2.723597	-1.630833
H	0.379170	-3.434010	-1.399300
C	0.760478	2.048840	2.342818
H	0.062894	2.327804	3.142240
H	1.761643	1.950392	2.771824
H	0.781888	2.843081	1.594031
C	4.893314	-1.779254	0.261519
H	5.628320	-1.206989	0.858082
H	4.955402	-2.817693	0.629831
C	3.026132	-1.094812	1.838785
H	3.699641	-0.541586	2.517253
H	0.526465	0.020768	2.377260
H	2.695790	-2.026915	2.325327
C	4.440608	2.215365	0.645180
H	3.805915	2.379678	1.523945
H	4.819026	1.189494	0.684390
H	5.295004	2.895948	0.727037
C	5.290805	-1.735590	-1.215586
H	4.611317	-2.345956	-1.821464
H	5.256555	-0.709445	-1.598817
H	6.307352	-2.119836	-1.357456
H	-5.345330	-2.215194	1.763789

Si	-4.305694	-1.395857	1.075467
Si	-5.339384	0.219734	-0.318752
Si	-2.691874	-2.669758	-0.104358
Si	-2.898222	-0.235957	2.575706
H	-6.217108	1.091302	0.514359
H	-6.205496	-0.461891	-1.322959
Si	-3.736752	1.539165	-1.464505
Si	-1.151055	-0.969079	-0.752560
H	-2.091678	-3.659828	0.835911
H	-3.286663	-3.416969	-1.248346
H	-3.573111	0.823816	3.376459
H	-2.221769	-1.173156	3.519162
Si	-1.323073	0.626774	1.024812
H	-4.428615	2.534742	-2.334332
Si	-2.241937	0.095171	-2.597142
Si	-2.262796	2.577609	0.075314
H	-1.302498	0.902764	-3.426629
H	-2.960551	-0.845796	-3.503421
H	-1.249016	3.391326	-0.653103
H	-2.928224	3.451676	1.081104

4d-ts

Hf	1.880618	-0.022780	-0.006819
N	0.563627	-0.699396	-1.468856
N	3.174226	-1.442870	0.513832
N	0.476006	0.535775	1.691279
N	2.930956	1.623112	-0.669972
C	4.208911	2.191125	-0.239858
H	4.984140	1.992506	-1.001932
H	4.111306	3.289455	-0.191373
C	2.421682	2.348572	-1.838517
H	1.474989	1.922195	-2.186769
H	2.245385	3.411316	-1.605242
H	3.132127	2.310090	-2.681359
C	0.930376	-1.392502	-2.713764
H	0.513036	-0.890851	-3.599373
H	2.019340	-1.415085	-2.838546
H	0.582197	-2.435514	-2.722807
C	0.820604	1.477718	2.774219
H	0.174175	1.344294	3.652030
H	1.853550	1.301799	3.098932
H	0.745814	2.520339	2.443796
C	4.328807	-2.298815	0.357063
H	5.043051	-2.117419	1.180618
H	4.023978	-3.355214	0.449023
C	2.352272	-1.533540	1.726447

H	2.918938	-1.322233	2.648722
H	1.154051	-0.508066	1.884637
H	1.832824	-2.499780	1.833174
C	4.693014	1.684577	1.118723
H	3.982571	1.948995	1.911373
H	4.822336	0.598151	1.120799
H	5.655041	2.143728	1.371048
C	5.029000	-2.082527	-0.985156
H	4.355204	-2.312929	-1.818300
H	5.360770	-1.043954	-1.092884
H	5.907559	-2.731106	-1.072078
H	-4.985212	-2.906431	1.127709
Si	-4.071050	-1.809256	0.694518
Si	-5.339458	0.036821	-0.078927
Si	-2.485278	-2.479253	-0.931650
Si	-2.618444	-1.063405	2.403532
H	-6.234386	0.510798	1.016355
H	-6.209859	-0.389730	-1.212551
Si	-3.946753	1.813668	-0.799503
Si	-1.136494	-0.520513	-1.073829
H	-1.723023	-3.652295	-0.413595
H	-3.111059	-2.869885	-2.227245
H	-3.322585	-0.384654	3.528655
H	-1.844386	-2.208014	2.964127
Si	-1.218764	0.401153	1.157168
H	-4.782372	2.953947	-1.278217
Si	-2.419309	0.989398	-2.404799
Si	-2.439208	2.424407	0.919703
H	-1.589353	2.111548	-2.933098
H	-3.097822	0.338045	-3.561922
H	-1.569195	3.541446	0.449730
H	-3.102750	2.858380	2.181661

4e: H-Hf-MeN-Si

Hf	2.113743	-0.199907	-0.448173
N	0.931273	-1.692233	0.320110
N	4.002659	-0.146888	0.322763
N	0.975344	1.490904	-0.684272
C	1.261164	-3.012764	0.872122
H	0.955076	-3.102211	1.924168
H	2.340618	-3.195390	0.830626
C	1.369426	2.822270	-1.164546
H	1.207258	3.597052	-0.401955
H	2.432091	2.842390	-1.435246
H	0.807183	3.110247	-2.063547
C	4.848162	0.809090	1.028086

H	5.191496	0.358215	1.975393
H	5.759509	1.005451	0.437210
C	4.691174	-1.425369	0.123004
H	4.949997	-1.906250	1.079930
H	4.066906	-2.129169	-0.447797
H	5.616806	-1.298453	-0.458658
C	4.148870	2.132242	1.332609
H	3.858488	2.654864	0.415327
H	3.249944	1.977743	1.940481
H	4.819109	2.794839	1.889967
H	-4.749214	-0.786940	-2.720324
Si	-3.751366	-0.475653	-1.654882
Si	-4.883061	0.156535	0.329828
Si	-2.213727	1.219754	-2.258580
Si	-2.263592	-2.258500	-1.193194
H	-5.785042	-0.949820	0.762870
H	-5.738844	1.347529	0.057334
Si	-3.369497	0.664667	2.081551
Si	-0.729306	1.134573	-0.398789
H	-1.528375	0.856414	-3.531439
H	-2.859295	2.551527	-2.439670
H	-2.945662	-3.443765	-0.598664
H	-1.583754	-2.691141	-2.447048
Si	-0.762027	-1.183468	0.306059
H	-4.121183	1.049324	3.312000
Si	-1.833177	2.308700	1.354298
Si	-1.885140	-1.147556	2.404738
H	-0.896699	2.651546	2.464429
H	-2.486270	3.568575	0.897182
H	-0.950688	-0.839657	3.526646
H	-2.577413	-2.429600	2.720363
H	2.401562	-0.762035	-2.182954
H	0.771666	-3.820008	0.309545

4e-ts

Hf	-1.819791	-0.109926	-0.270730
N	-0.555887	-1.472446	0.689848
N	-3.569499	-1.766477	-0.021341
N	-0.454403	0.961980	-1.422933
N	-2.755689	1.166403	1.042107
C	-3.182892	2.561286	0.958760
H	-4.234090	2.628137	1.293374
H	-2.602741	3.170446	1.673937
C	-2.937804	0.667060	2.407462
H	-2.642142	-0.384112	2.491640
H	-2.332572	1.236838	3.130431

H	-3.991410	0.745016	2.724517
C	-0.894933	-2.620060	1.548691
H	-0.582107	-2.457892	2.591592
H	-1.973937	-2.797496	1.537616
H	-0.404916	-3.541731	1.200181
C	-0.682771	1.759901	-2.639388
H	-0.117118	1.361224	-3.494568
H	-1.740642	1.748501	-2.914979
H	-0.380692	2.809491	-2.504971
C	-4.955052	-1.514095	0.432275
H	-5.526477	-2.439370	0.275582
H	-4.910096	-1.353322	1.512429
C	-3.397812	-2.044706	-1.280419
H	-4.213914	-2.129672	-2.004807
H	-2.728803	-0.311065	-1.986222
H	-2.435901	-2.437938	-1.610223
C	-3.063983	3.177840	-0.432038
H	-2.021821	3.228742	-0.755913
H	-3.629057	2.602477	-1.175402
H	-3.465389	4.196749	-0.423957
C	-5.684272	-0.339152	-0.231442
H	-5.166412	0.602388	-0.033595
H	-5.766145	-0.464080	-1.315929
H	-6.699652	-0.268326	0.173194
H	5.306718	-1.910642	-2.023885
Si	4.262448	-1.194202	-1.233183
Si	5.292245	0.167023	0.412072
Si	2.688745	-2.631041	-0.204587
Si	2.799080	0.114200	-2.553982
H	6.213441	1.133997	-0.253435
H	6.122281	-0.687246	1.310791
Si	3.695039	1.352243	1.702805
Si	1.147852	-1.024511	0.643052
H	2.063538	-3.507905	-1.238532
H	3.284964	-3.511331	0.841216
H	3.481760	1.249182	-3.238841
H	2.179028	-0.747721	-3.603068
Si	1.219378	0.792862	-0.906173
H	4.399450	2.188903	2.719600
Si	2.151434	-0.185100	2.632940
Si	2.272335	2.580913	0.261591
H	1.167265	0.548953	3.482698
H	2.806481	-1.218525	3.486105
H	1.296895	3.365618	1.073985
H	3.014838	3.538334	-0.608674

$CH_3CH=NCH_3$ onto H-Si(100) product with C-Si bond:

N	-3.772645	0.328150	0.405065
C	-3.074273	-0.729713	-0.291298
H	-3.442513	-0.728444	-1.325936
C	-4.612147	1.282725	-0.279160
H	-5.436444	0.797062	-0.827064
H	-5.058070	1.960363	0.454584
H	-4.053518	1.902901	-0.997670
C	-3.356532	-2.115243	0.315397
H	-3.016975	-2.166411	1.356660
H	-4.433998	-2.318793	0.305864
H	-2.845596	-2.909677	-0.239686
H	1.982995	3.600382	-0.670031
SI	1.477953	2.226939	-0.376506
SI	3.084159	0.607799	-1.024087
SI	-0.611152	1.745296	-1.374083
SI	0.889923	1.891718	1.886933
H	4.355813	0.843958	-0.280810
H	3.384244	0.759356	-2.477494
SI	2.315198	-1.595475	-0.603202
SI	-1.154954	-0.350279	-0.404923
H	-1.585530	2.810279	-0.999446
H	-0.556839	1.682190	-2.862963
H	2.045219	1.925116	2.827555
H	-0.088173	2.931059	2.320160
SI	-0.109185	-0.250406	1.755868
H	3.344057	-2.589781	-1.028787
SI	0.199701	-1.891698	-1.613532
SI	1.685159	-1.792042	1.665787
H	-3.701730	0.371328	1.407968
H	-1.056235	-0.521668	2.879331
H	-0.252380	-3.301217	-1.418720
H	0.201815	-1.618978	-3.079664
H	1.232946	-3.184304	1.951616
H	2.771901	-1.454305	2.627892

$CH_3CH=NCH_3$ onto H-Si(100) Forming C-Si ts:

N	-3.92221600	0.41278600	0.40160400
C	-4.58843800	-0.50907400	-0.19259400
H	-5.33274500	-0.18447200	-0.91959600
C	-3.99659600	1.84611700	0.10941500
H	-4.04756800	2.39932100	1.04898600
H	-3.09047900	2.12746500	-0.43603500
H	-4.87752000	2.05190300	-0.49986900
C	-4.37302800	-1.95496700	0.02953900
H	-3.71625800	-2.15595700	0.87720100

H	-5.33384200	-2.46523200	0.15643500
H	-3.89478500	-2.35098600	-0.87765600
H	2.46685400	3.47336900	-0.29348200
Si	1.81700900	2.12763800	-0.20747100
Si	3.45881200	0.41976500	-0.12206700
Si	0.16780900	1.60462800	-1.82378000
Si	0.43772700	1.90080000	1.69125200
H	4.36771200	0.64661000	1.04208100
H	4.31090700	0.49146900	-1.34657100
Si	2.46407200	-1.72868200	0.00432500
Si	-0.98560300	-0.40339200	-1.22401200
H	-0.77354200	2.77989100	-1.82401900
H	0.73493000	1.56773400	-3.20703000
H	1.12875200	1.92839000	3.01370800
H	-0.59047900	2.99082300	1.72058800
Si	-0.53582400	-0.19424100	1.16110800
H	3.52544900	-2.78345800	0.04505600
Si	0.81533000	-1.90688800	-1.68307800
Si	1.03487000	-1.80839100	1.88280800
H	-3.14603800	0.12138300	1.02487700
H	-1.81821900	-0.32968400	1.98912200
H	0.35354500	-3.33340100	-1.68801500
H	1.41134500	-1.67634700	-3.03560000
H	0.42195100	-3.16487900	2.01994900
H	1.66508800	-1.47320700	3.19330500

$CH_3CH=NCH_3$ onto H-Si(100) product with N-Si bond:

N	2.904404	-0.355192	0.193569
C	3.890088	0.145824	-0.773580
H	4.271432	-0.686553	-1.391331
C	3.377368	-1.499059	0.973460
H	4.272152	-1.238969	1.551149
H	2.614482	-1.814783	1.690394
H	3.626093	-2.365397	0.336732
C	5.068315	0.884637	-0.126634
H	4.711536	1.734638	0.463894
H	5.651561	0.232801	0.531486
H	5.746235	1.259728	-0.901908
H	-2.978481	-2.669784	-1.594557
SI	-2.102873	-1.649687	-0.946655
SI	-2.978221	0.521742	-1.312659
SI	0.157092	-1.728187	-1.636001
SI	-1.796953	-1.998746	1.370884
H	-4.358606	0.609082	-0.754356
H	-3.072389	0.782698	-2.778245
SI	-1.620556	2.182515	-0.304630

SI	1.185780	-0.180232	-0.125927
H	0.671547	-3.117701	-1.452036
H	0.348578	-1.363368	-3.069655
H	-3.033758	-1.826506	2.184026
H	-1.275500	-3.375351	1.610879
SI	-0.162318	-0.356957	1.858488
H	-2.178407	3.540381	-0.571174
SI	0.622658	1.946930	-1.017470
SI	-1.338386	1.695077	1.989780
H	3.385932	0.832151	-1.463298
H	0.627522	-0.658376	3.087826
H	1.452622	3.033808	-0.421457
H	0.781914	2.009564	-2.498380
H	-0.520371	2.758725	2.639575
H	-2.616686	1.566774	2.744633

$CH_3CH=NCH_3$ onto H-Si(100) Forming N-Si ts:

N	-3.22047900	-0.21050200	-0.15327600
C	-3.99063800	1.01019900	0.07300900
H	-4.69056500	0.85368500	0.90266000
H	-3.32089300	1.83533100	0.31964900
H	-4.56515400	1.28940000	-0.81783100
C	-3.72708600	-1.40893900	0.12627500
H	-4.66543300	-1.47168200	0.68520100
H	-1.89498800	-1.81097000	0.72100800
H	-0.16817800	3.28897800	1.86422400
Si	0.75823400	2.14758100	1.60529200
Si	1.34531100	2.06796800	-0.68219500
H	1.90893900	2.27135100	2.54511000
Si	-0.35068000	0.06460800	1.83128400
Si	2.88183900	0.29323000	-1.01060100
H	1.94988500	3.34207300	-1.17248200
Si	-0.78048800	1.54884000	-1.58695000
Si	1.30491500	-1.62541100	1.91407800
Si	-1.39313500	-0.43093400	-0.26123800
H	-1.34310200	0.00257500	2.94204800
H	4.12761000	0.54988400	-0.23020400
H	3.26750700	0.22344300	-2.45004000
Si	1.94820100	-1.78548900	-0.35581100
H	-1.62057800	2.77764400	-1.40711800
H	-0.70828700	1.30206500	-3.05856500
H	0.75494200	-2.91189900	2.42368200
H	2.44191600	-1.22834400	2.79348200
Si	-0.10786100	-2.00769700	-1.51031000
H	-3.43158100	-2.29563200	-0.41559400
H	2.91781400	-2.89275400	-0.61338200

H	-0.65919300	-3.38955000	-1.40641300
H	0.06032000	-1.68741200	-2.95789300