Electronic Supplementary Material (ESI) for Dalton Transactions.

Preparation of monopodal and bipodal aluminum surface species by selective protonolysis of highly reactive [AlH_3NMe_2Et] on silica

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Electronic Supplementary Information

General Procedures.

All experiments were carried out under controlled atmosphere, using Schlenk and glove box techniques for the organometallic synthesis. For the synthesis and treatments of the surface species, reactions were carried out using high-vacuum lines (1.34 Pa) and glove box techniques. Benzene was distilled on Na-benzophenone and degassed through freeze pump thaw cycles. Infrared spectra were recorded on a Nicolet Magna 5700 FT spectrometer equipped with a cell designed for *in situ* reactions under controlled atmosphere. Infrared spectra (DRIFT) were recorded on a Nicolet Magna 6700 FT spectrometer equipped with a cell under controlled atmosphere. Elemental analyses were performed at the Mikroanalytisches Labor Pascher, Remagen (Germany). ^{1}H MAS and ^{13}C CP-MAS solid-state NMR spectra were recorded on a Bruker DSX-300 spectrometer. For specific studies (see below), ^{1}H MAS and ^{13}C CP-MAS solid-state NMR spectra were recorded on Bruker Avance-500 spectrometers with a conventional double-resonance 4 mm CP-MAS probe and on a Avance III 800 spectrometer (^{1}H: 800.13 MHz, ^{13}C: 201.21 MHz, ^{27}Al: 208.50 MHz). The samples were introduced under Ar in a zirconia rotor, which was then tightly closed. In all experiments, the rotation frequency was set to 10 kHz unless otherwise specified. Chemical shifts were given with respect to TMS as external reference for ^{1}H and ^{13}C NMR. ^{27}Al MAS NMR spectra at 18.8 T were acquired at a spinning frequency of 20 kHz in 3.2 mm rotors. D-HMQC experiments were set up with a ^{27}Al spin echo selective to the central transition, with pulses of 7.25 and 14.5 μs, and a ^{1}H $\pi/2$ pulse of 3 μs on either side of the ^{27}Al π pulse. A recycling delay of 2 s was used. The number of scans for each t_1 increment was set to 2048. The $SR4^2_1$ dipolar recoupling scheme was applied for 500 μs. The ^{1}H MAS NMR spectrum acquired with a *J*-HMQC ^{27}Al filtering was obtained with recycling delay of 1 ms.

Preparation and Characterization of silica and materials 1 and 2

Sylopol SY2408 Silica from Grace Davidson with a specific area of 300 m².g.-1 ((Pore volume: 1.55 mL.g^{-1}; particle size: 40 µm) was selected as a support for grafting of Al compounds. Isolated and vicinal surface silanols were dehydroxylated under high vacuum at 473K (Sylopol$_{200}$) or 973 K (Sylopol$_{700}$) for 15 h. The titration by EtMgBr showed that the silica supports presented 1.62 mmol$_{OH}$.g^{-1} (Sylopol$_{200}$) and 0.6 mmol$_{OH}$.g^{-1} (Sylopol$_{700}$) respectively.

Using the double Schlenk technique, Sylopol$_{700}$ and Sylopol$_{200}$ were treated with excess [(AlH_3)($EtMe_2N$)] in benzene (10 mL) for 2 h at room temperature. After repeated washings with benzene (10 mL), followed by evacuation of the volatile under high vacuum (10^{-5} mmHg), **1** and **2** were afforded as a white powder and characterized by DRIFTS, solid-state NMR spectroscopy and mass-balance analysis.

Hydrolysis of the synthesized materials was performed in a closed glass vessel with a determined volume (typically 500 mL). A known quantity of the sample (about 35 mg) was introduced into the glass vessel in the glovebox. Then, the vessel was evacuated under high vacuum and an excess of oxygen-free water vapor was introduced at ambient temperature. The hydrogen evolved was quantified by a calibrated GC (HP 6890) equipped with 15 m HP PLOT MoleSieve 5Å column and TCD.

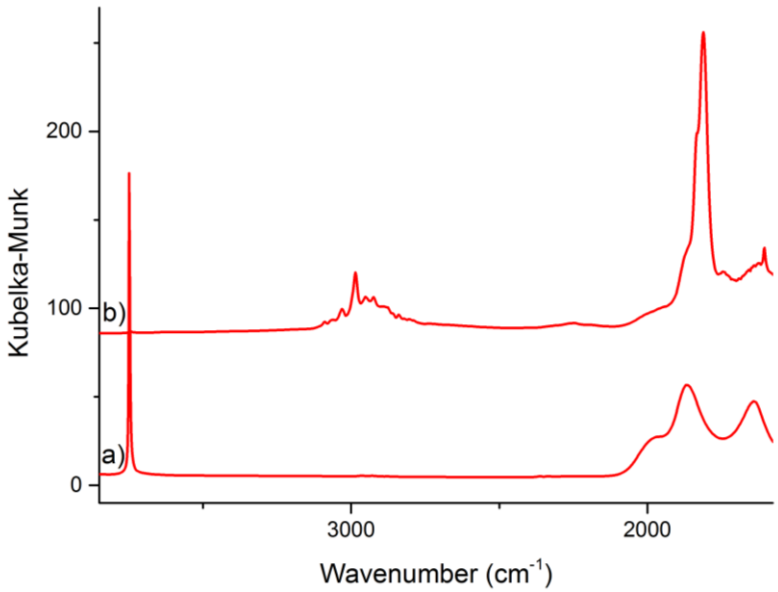


Figure S1. DRIFT spectra of (a) Sylopol-$_{700}$ and (b) material **2**

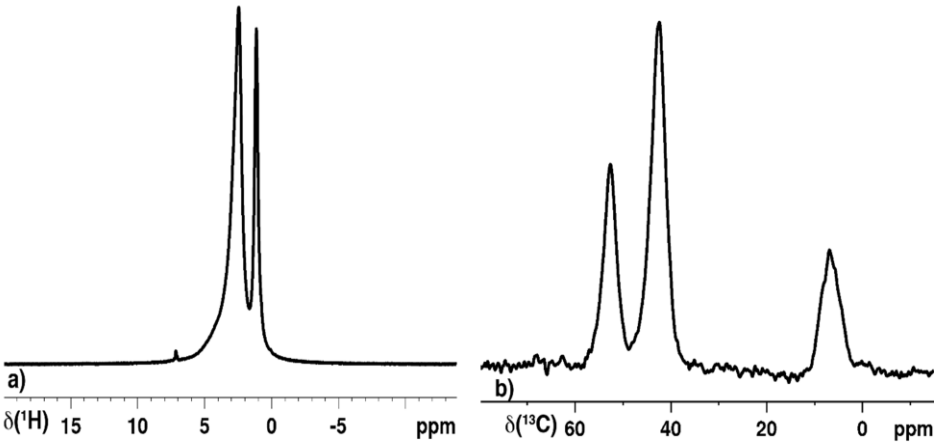
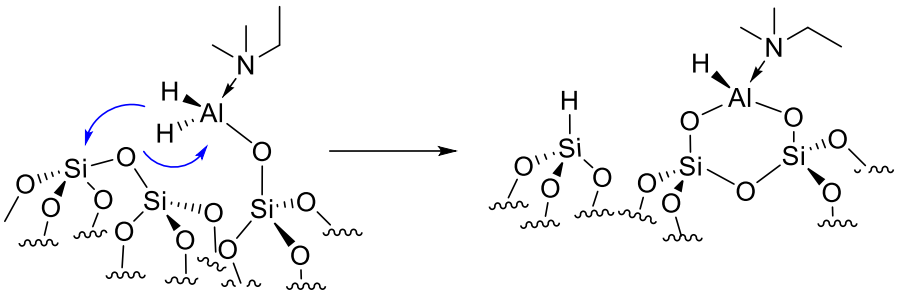


Figure S2. ^{1}H (a) and ^{13}C CP (b) MAS NMR spectra **1** (18.8 T).

Table S1. Mass Balance Analysis Data for **1** and **2**

Material	wt % Al [a]	wt %C[a]	wt %N[a]	C/N	C/Al	N/Al	H_2/Al Hydrolysis[b]
1	2.69	4.71	1.45	3.8	4.4	1.1	1.1
2	1.89	3.03	1.12	3.0	3.6	1.2	1.5

[a] Percentage determined by elemental analysis. The error is <5%. [b] See the Experimental Section.



Scheme S1. Formation of bipodal species by opening of siloxane bridges of $SiO_{2\text{-}700}$

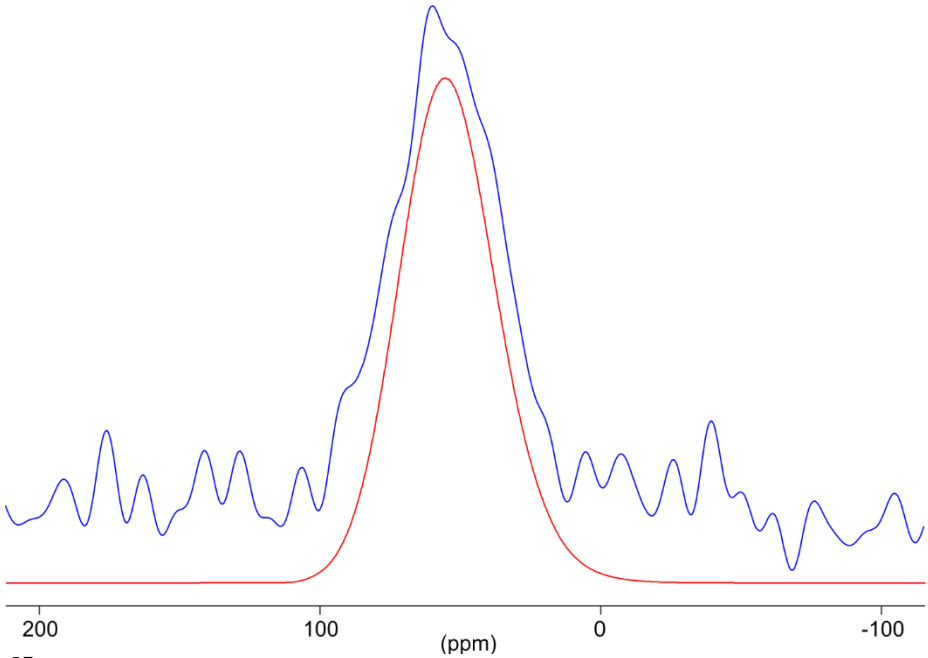


Figure S3. ^{27}Al echo MAS NMR spectrum of **1** (blue trace, 18.8 T, spinning speed 20 kHz) and best fit simulation (red trace, from the Dmfit program[1a], with a CzSimple model, with chemical shift of 65 ppm, quadrupolar coupling constant of 8.2 MHz, chemical shift full width at half maximum of 35 ppm)

The lineshape of the ^{27}Al signal is non-symmetrical, which is often related to either quadrupolar coupling constant (C_Q) and/or chemical shift (CS) distributions. A typical approach to get best-fit simulations of such spectra is by using the Czjzeck model.[1b] In the present case, combination of both C_Q and CS Czjzeck distributions must be resorted to, in order to account for the ^{27}Al NMR signal dissymmetry. Thus, the ^{27}Al MAS NMR signal of **1** corresponds to a single type of Al center, featuring CS of 65 ppm (distinct from the signal maximum, due to quadrupolar coupling influence), with a distribution of about 35 ppm, and a C_Q of about 8 MHz). Such large chemical shift distribution can be directly linked to the geometrical parameters (bond distances and angles) distribution of the Si-O-Al-O-Si framework, due to silica surface heterogeneity.

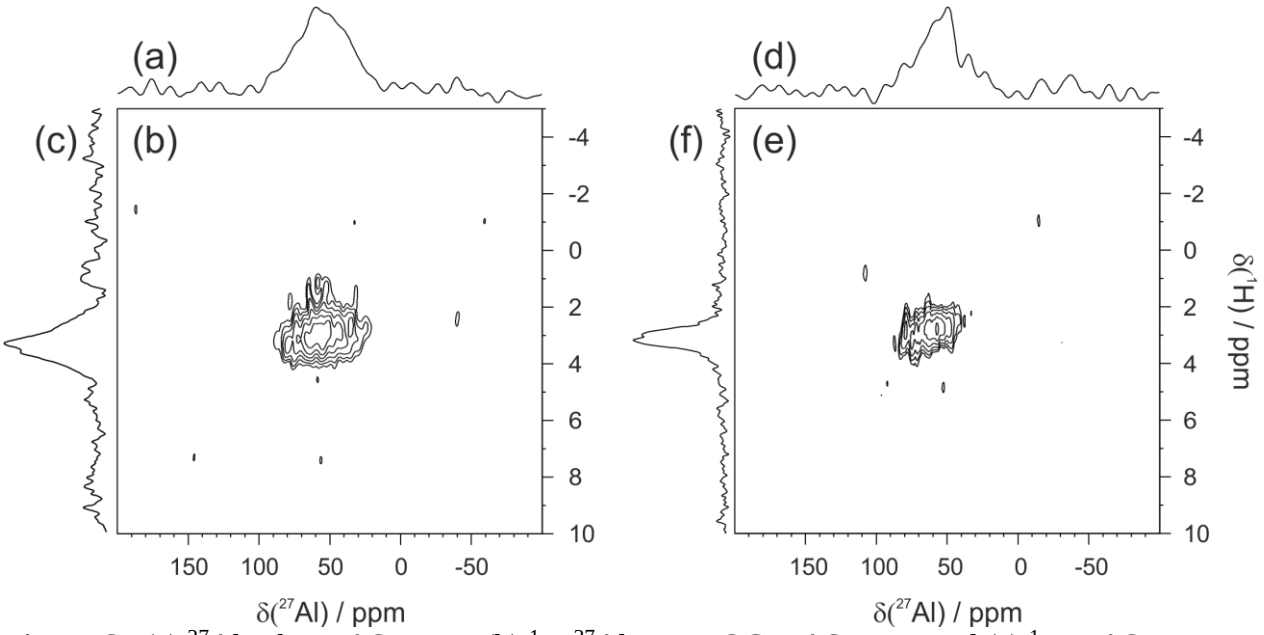


Figure S4 (a) ^{27}Al echo MAS NMR, (b) ^{1}H-^{27}Al D-HMQC MAS NMR and (c) ^{1}H MAS NMR recorded with a *J*-HMQC ^{27}Al filter of **1**; (d) ^{27}Al echo MAS NMR, (e) ^{1}H-^{27}Al D-HMQC MAS NMR and (f) ^{1}H MAS NMR recorded with a *J*-HMQC ^{27}Al filter of **2** (18.8 T, spinning speed 20 kHz)

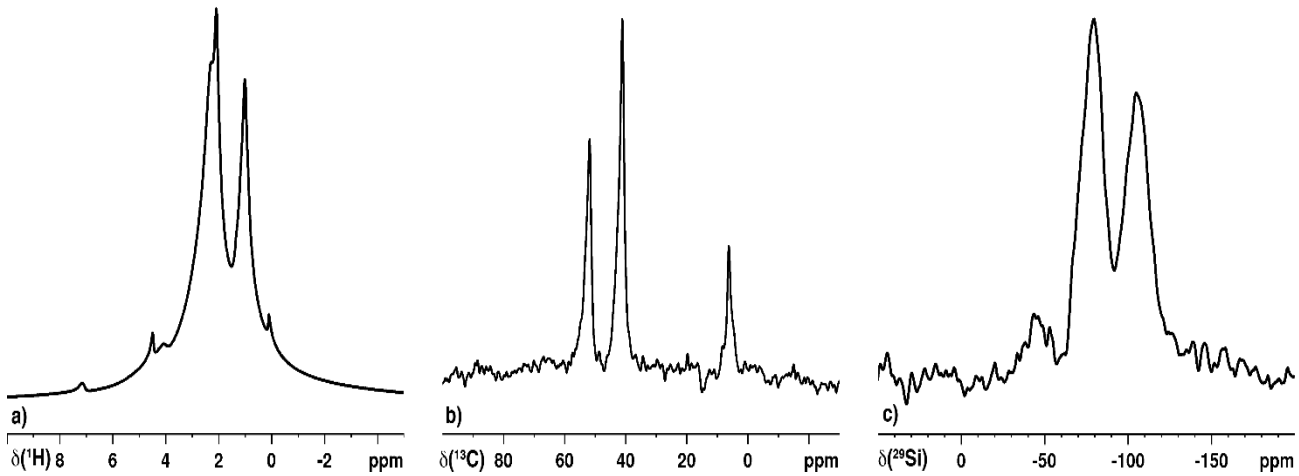


Figure S5. ^{1}H MAS (a) ^{13}C CP/MAS-NMR (b) ^{29}Si CP/MAS-NMR (c) of **2**

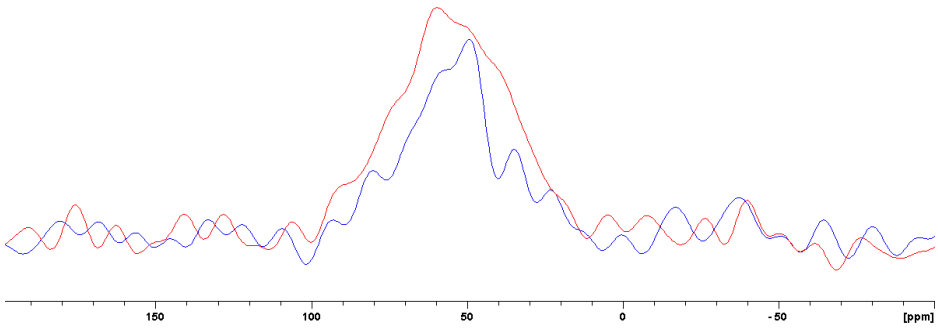


Figure S6. ^{27}Al echo MAS NMR spectrum of **1** (red trace) and **2** (blue trace) (18.8 T, spinning speed 20 kHz)

Figure S7. Energy profiles

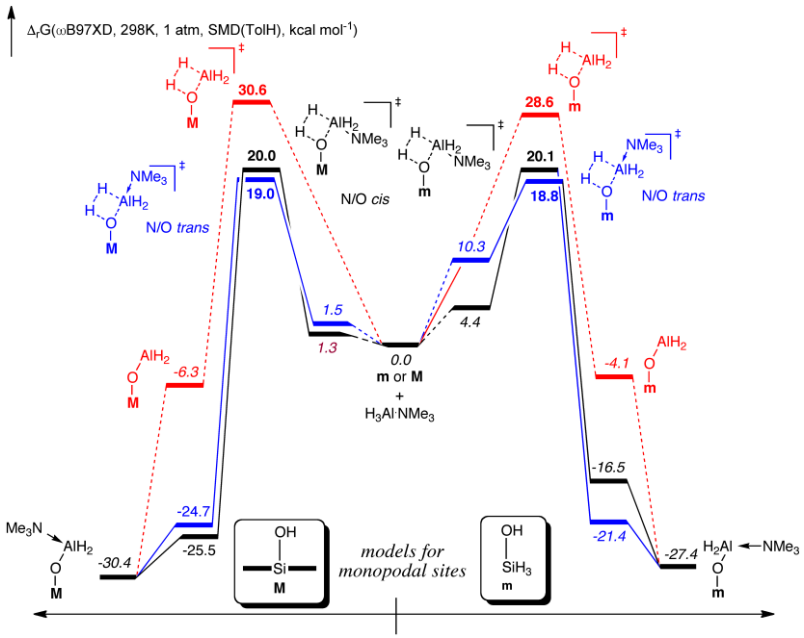


Figure S7a. Gibbs energy profile for the functionalization of monopodal sites by $AlH_3.NMe_3$. **m** refers to the minimalist H_3SiOH model, **M** refers to a silica cluster that shows an isolated silanol group.

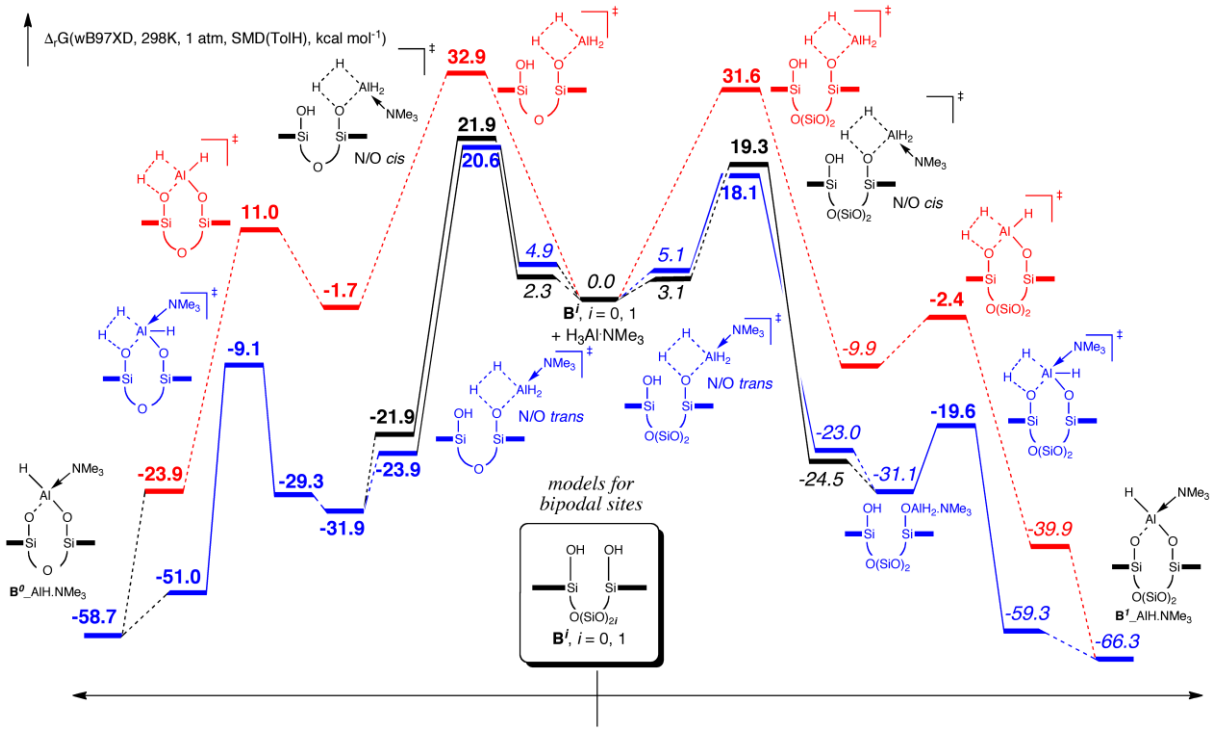


Figure S7b. Gibbs energy profile for the functionalization of bipodal sites by $AlH_3.NMe_3$ depending on the cycling strain between the two silanol groups.

Computational Details

The electronic structure calculations for the depiction of minima and transition states molecular structures were performed at the density functional theory (DFT) level using the ωB97XD[2] hybrid functional as implemented in the Gaussian program code.[3] Silicon aluminium atoms were described by the corresponding scalar relativistic pseudopotentials of the Stuttgart-Dresden-Koln type[4] in association with their polarized basis set (α_d(Si) = 0.284 ; α_d(Al) = 0.190).[5] For the rest atoms the polarized all-electron triple zeta basis set 6-311G(d,p) was used.[6] Optimization were carried without any geometry constraint. Enthalpy energies were obtained at T = 298.15K based on the harmonic approximation. Solvation by toluene was taken into account in all calculations, including optimizations and frequency calculation, by the SMD implicit solvent model.[7] Intrinsic Reaction Paths (IRPs) were traced from the various transition structures to verify the reactant to product linkage.[8]

References

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Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
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Cartesian Coordinates & Energies

Precursors

NMe_3

E: -174.468415509 ; H: -174.341312 ; G: -174.374945
N -0.11267145 -1.67982610 0.00322245
C 0.32466180 -0.98226633 1.19577505
H 0.05603054 0.07553284 1.12990713
H -0.16863875 -1.40178667 2.07677783
H 1.41868429 -1.04766587 1.35371163
C 0.17549137 -3.09749625 0.08949606
H -0.31659139 -3.52694749 0.96632561
H -0.20662712 -3.61071174 -0.79714284
H 1.25954303 -3.30950179 0.16769116
C 0.47162775 -1.09891400 -1.18889582
H 0.08084623 -1.59945439 -2.07890825
H 0.20997531 -0.03948016 -1.25650183
H 1.57582291 -1.18024855 -1.20836667

AlH_3

E: -3.78198739162 ; H: -3.759937 ; G: -3.785205
Al 0.12904135 -0.22357992 0.09530194
H -0.13692014 0.23745865 1.59240129
H 1.45508751 0.23206644 -0.65256973
H -0.93190110 -1.13848416 -0.65487207

$Me_3N{\cdot}AlH_3$

E: -178.310632460 ; H: -178.157273 ; G: -178.197119
C 0.45181643 -0.98905958 1.21692836
H 0.19910008 0.07004886 1.14987439
H -0.02896518 -1.41351561 2.09939760
H 1.53854975 -1.09598487 1.31202613
C 0.29692443 -3.12345829 0.09675752
H -0.18418576 -3.55356684 0.97619100
H -0.07090108 -3.63417875 -0.79421582
H 1.38106773 -3.26505060 0.17357649
C 0.59724069 -1.10287164 -1.19137865
H 0.21625704 -1.60580828 -2.08117059
H 0.35082043 -0.04199027 -1.25188458
H 1.68624123 -1.21941168 -1.14857281

N -0.03061819 -1.68704007 0.00953824
H -2.56197647 -2.14672038 1.25480986
H -2.22605609 0.12981437 -0.22986052
H -2.39288212 -2.30431206 -1.47319274
Al -2.08887012 -1.47149940 -0.12842320

Al_2H_6
E: -7.61873483477 ; H: -7.570068 ; G: -7.602802
Al -0.04071229 -0.26715849 0.21053184
H 1.09808393 0.64444139 0.81624632
H -1.09656380 0.09035718 -0.90806083
H 0.62149639 -1.85427930 -0.11994667
Al -0.19483763 -2.68564295 1.18628698
H -1.33350804 -3.59753090 0.58083587
H -0.85688151 -1.09851193 1.51599339
H 0.86082505 -3.04289581 2.30515647

H_2
E: -1.17561833209 ; H: -1.162226 ; G: -1.177023
H 0.00000000 0.00000000 0.02759597
H 0.00000000 0.00000000 0.77240403

Silica models and grafted complexes

Monopodal site m
m
E: -81.5455501204 ; H: -81.502421 ; G: -81.531720
Si -0.06934056 0.77773319 -0.01628962
H 0.46156636 -0.61227121 -0.08150333
H 0.41305888 1.45213836 1.23059536
H -1.56621967 0.75182097 0.01850576
O 0.50638618 1.54548996 -1.40058299
H 0.25045585 2.46146796 -1.51033418

$H_3SiOH_AlH_3{\cdot}NMe_3$_TS_HH (N/O *trans*) adduct
E: -259.858895341 ; H: -259.659509 ; G: -259.712393
Si -2.68789919 -1.88154558 -0.61169623
H -1.93626797 -3.02915950 -0.03121710
H -2.33398955 -1.63799791 -2.03142347
H -4.15664861 -2.11926989 -0.45509153
O -2.33462806 -0.42137165 0.21802631
N 1.86515448 0.89152812 0.27467078
C 2.39990106 0.91104177 -1.09106489
H 1.83309775 1.62772991 -1.68713147
H 3.46269167 1.18959572 -1.09663877
H 2.28235707 -0.07826141 -1.53582293
C 2.57807412 -0.09774265 1.08994361
H 3.64660327 0.14605093 1.16667893
H 2.13831336 -0.12134377 2.08809254
H 2.46260956 -1.08349138 0.63675895
C 1.96407475 2.22302605 0.88244921
H 1.52388611 2.19361234 1.88035708
H 3.01068019 2.54950098 0.95395955
H 1.40171809 2.93457855 0.27615162
H -0.37868217 0.41904986 1.80583657
H -0.62483796 1.59548634 -0.73018284
H 0.12081646 -1.08953301 -0.52037270
Al -0.25164483 0.32680203 0.18918173
H -2.69605856 -0.30865638 1.09807556

$H_3SiOH_AlH_3{\cdot}NMe_3$_TS_HH (N/O *trans*) TS

E: -259.842478494 ; H: -259.648135 ; G: -259.698880

Si	-4.00781430	0.19059783	1.00549421
H	-3.31071339	-0.94712520	1.68815311
H	-3.99926492	-0.04602857	-0.47013844
H	-5.41985839	0.24865643	1.49504675
O	-3.23521101	1.64570395	1.34093815
N	0.56116838	2.90255262	1.47422125
C	1.31429303	3.14800869	0.23281142
H	0.81417875	3.92460863	-0.34811524
H	2.33800136	3.47078418	0.45754826
H	1.35119193	2.23119387	-0.35794676
C	1.21829049	1.84294339	2.25492933
H	2.24616298	2.12863803	2.50999973
H	0.65939908	1.66713929	3.17545985
H	1.23662267	0.92001540	1.67338061
C	0.48884916	4.14077911	2.26540129
H	-0.07904914	3.95731388	3.17889661
H	1.49392313	4.48975004	2.53213587
H	-0.01781069	4.91369342	1.68576255
H	-1.64875010	2.20716862	2.69576536
H	-1.72653091	3.67731250	0.15884474
H	-0.84594618	0.95789712	0.14306701
Al	-1.40251949	2.28104356	0.86556897
H	-2.52567799	1.87526211	2.31506355

$H_3SiOH_AlH_3{\cdot}NMe_3$_TS_HH (N/O *trans*) product / H_2 adduct

E: -259.895875015 ; H: -259.699499 ; G: -259.755092

Si	-1.88473010	-1.75763310	0.48250251
H	-2.94918497	-1.49074611	1.50330367
H	-0.98342790	-2.83200173	1.02602968
H	-2.53782262	-2.29039674	-0.75920075
O	-1.01861085	-0.38440680	0.18501511
N	1.66499900	0.63996387	-0.11990808
C	2.57650656	1.44649506	-0.94906897
H	2.16156770	2.44860122	-1.06823976
H	3.56603712	1.51586489	-0.48219690
H	2.67252888	0.98511248	-1.93318714
C	2.17367548	-0.73759720	0.01314609
H	3.15244026	-0.74044272	0.50728170
H	1.46435294	-1.32161529	0.59988581
H	2.26461287	-1.18589964	-0.97714070
C	1.50865057	1.25097113	1.21403282
H	0.80327658	0.65557065	1.79326261
H	2.47456839	1.29658393	1.73085079
H	1.10523819	2.25823969	1.10268208
H	-1.92888383	1.75104270	2.39908076
H	-0.56817838	2.14130850	-1.03983680
H	0.14980225	-0.17052870	-2.40421901
Al	-0.19913648	0.58557545	-1.03530647
H	-1.75041055	1.25971285	1.86487785

$H_3SiOH_AlH_3{\cdot}NMe_3$_TS_HH (N/O *cis*) adduct

E: -259.866959418 ; H: -259.667655 ; G: -259.721803

Si	-0.84900945	-0.58519395	-2.65440153
H	0.37065943	-1.39752652	-2.33895995
H	-2.06997763	-1.39335867	-2.37319355
H	-0.80123733	-0.21024265	-4.10196924
H	-0.24545609	1.41734552	-1.79701654
O	-0.95097672	0.76865877	-1.65861401
H	3.61720096	1.18978908	-2.15710494
H	3.30384244	3.74725242	-1.17947136
H	1.14975313	2.31623440	-1.99909798
Al	2.67844212	2.29818993	-1.47281184
N	2.44702408	1.53909499	0.43268379
C	1.86065503	0.18466691	0.35258239
H	1.77046681	-0.25177908	1.35363949

H	0.87082227	0.24663049	-0.10042982
H	2.49866011	-0.45235340	-0.26160412
C	3.77388751	1.47061433	1.07774453
H	4.20881742	2.46973259	1.12962524
H	3.68306793	1.06321541	2.09088491
H	4.43005579	0.82728375	0.48961818
C	1.55540946	2.42215361	1.21221966
H	1.42202096	2.02848610	2.22596226
H	1.98967294	3.42118657	1.26830019
H	0.58255082	2.48308241	0.72273925

$H_3SiOH_AlH_3{\cdot}NMe_3$_TS_HH (N/O *cis*) TS

E: -259.840696035 ; H: -259.646352 ; G: -259.696734

Si	-0.63734776	0.19240659	-2.15522155
H	-0.06646318	-1.12528134	-2.56329902
H	-1.25309416	0.07237511	-0.80065989
H	-1.64542607	0.65548531	-3.14989108
H	1.01259701	1.85526136	-2.93424917
O	0.58978538	1.36015724	-2.05052949
H	3.65420080	0.99023055	-1.93599206
H	2.58687558	3.50214565	-1.06772131
H	1.97479298	2.41996197	-3.34240129
Al	2.44787535	2.00686008	-1.63581466
N	2.21855221	1.22980643	0.37929162
C	2.07799759	-0.23344983	0.39577874
H	2.10280475	-0.61762412	1.42309109
H	1.12859929	-0.52483136	-0.05410500
H	2.89140730	-0.68350865	-0.17502997
C	3.46773833	1.59910416	1.06701567
H	3.59074850	2.68273548	1.04430837
H	3.44796225	1.25926034	2.10962503
H	4.31525253	1.13805939	0.55687932
C	1.07941770	1.86261632	1.06213749
H	1.03040489	1.54900462	2.11242855
H	1.19111625	2.94683911	1.01704299
H	0.15055479	1.58555027	0.56364016

$H_3SiOH_AlH_3{\cdot}NMe_3$_TS_HH (N/O *cis*) product / H_2 adduct

E: -259.902743082 ; H: -259.708272 ; G: -259.762871

Si	-0.56581926	0.20118344	-2.50373167
H	0.20427042	-0.92408131	-3.13433037
H	-1.65574303	-0.40245365	-1.66627752
H	-1.21314894	0.98608675	-3.60696266
H	1.03720247	2.49183732	-4.11139033
O	0.39491730	1.15761270	-1.56794474
H	3.18911786	0.83652983	-2.00372208
H	2.21798744	3.30776044	-1.22788247
H	1.71541699	2.52332634	-4.42017970
Al	2.04357624	1.71695323	-1.30236073
N	2.25447939	1.19365769	0.67978929
C	2.07002643	-0.26329281	0.82404831
H	2.19305950	-0.56198808	1.87121505
H	1.06967235	-0.53281130	0.48475383
H	2.80589486	-0.78602015	0.21100832
C	3.60489491	1.57905021	1.12936605
H	3.74366868	2.65209369	0.98677880
H	3.74223555	1.33680224	2.18910169
H	4.35122245	1.04407181	0.53972977
C	1.23209880	1.90934238	1.46878546
H	1.30664956	1.63891280	2.52814174
H	1.37866623	2.98476278	1.35986784
H	0.24320581	1.64822666	1.09112111

$H_3SiO\_AlH_2{\cdot}NMe_3$

E: -258.725616216 ; H: -258.544992 ; G: -258.595532

Si	-0.14915944	0.57225318	-4.33979760
H	0.82232577	-0.54046770	-4.61302413
H	-1.51282102	-0.03254292	-4.18371037
H	-0.17729053	1.45720574	-5.55403910
O	0.27206473	1.44951274	-3.01208129
H	2.59775885	0.62017287	-1.60593862
H	0.54060476	1.83834785	-0.21777992
Al	1.31114038	1.58133004	-1.59906622
N	2.15118858	3.42579365	-1.95690236
C	3.08098577	3.74147319	-0.85641227
H	3.54194773	4.72352176	-1.01084739
H	2.53706102	3.74598526	0.08964093
H	3.86268777	2.98141397	-0.81274678
C	2.87976547	3.38831215	-3.24007507
H	2.18072050	3.14837739	-4.04145394
H	3.34667489	4.35887953	-3.44192424
H	3.65148661	2.61808849	-3.19937021
C	1.07686884	4.43681000	-2.02153628
H	1.49708135	5.42602208	-2.23489604
H	0.37263690	4.15974045	-2.80640695
H	0.54907308	4.46745029	-1.06732517

Monopodal site M

M

E: -1577.76577085 ; H: -1577.421077 ; G: -1577.559994

O	-0.20157562	0.54017456	3.98998270
Si	-0.38689758	0.77689533	2.38875611
O	0.70184947	1.90846992	1.87724372
Si	1.57843847	2.35772877	0.55602822
O	2.96124684	3.06163529	1.05272238
O	-0.12847776	-0.63734878	1.58417525
Si	-0.57608975	-1.48948460	0.24691140
O	-0.50361019	-3.08792200	0.55504245
O	-1.91968315	1.29919226	2.08706918
Si	-2.80680825	2.23017503	1.05770246
O	-1.86607620	3.44864444	0.45968489
Si	-0.84162087	3.81213621	-0.77971173
O	-1.27599418	2.95723547	-2.12484243
Si	-1.02247633	1.54083537	-2.92713727
O	0.50660118	1.00898258	-2.62325829
Si	1.39406529	0.08470004	-1.58755914
O	1.94163111	1.02693942	-0.35237857
O	0.45179203	-1.13506899	-0.99105516
O	-2.12263790	-1.08400806	-0.17210693
Si	-2.99421185	-0.02711406	-1.09537082
O	-2.11174266	0.41120285	-2.41272245
O	2.66950328	-0.55455088	-2.37399008
O	-4.07790340	2.87041810	1.85140100
O	-3.36584424	1.29406233	-0.17902115
O	0.69820624	3.41854226	-0.34726468
O	-4.35986452	-0.73434474	-1.67114866
O	-0.93710715	5.40539132	-1.10549430
O	-1.20902299	1.78999783	-4.52538043
Si	-4.52091264	4.40211456	2.40997592
H	-5.04393733	-0.92453263	-1.02796687
Si	-1.15468701	6.34842973	-2.48991557
Si	-2.11872223	1.12271794	-5.78279377
Si	0.91328304	1.01200223	5.16903678
Si	-1.61653625	-4.30571772	0.91869785
H	-0.82761290	-5.46865732	1.41060273
H	-2.55774443	-3.82556507	1.97250811
H	-2.37291275	-4.66824461	-0.31478700
H	0.53592514	0.28996503	6.41599860
H	2.28972559	0.62877098	4.74004555
H	0.82958806	2.48718693	5.37201398
H	-1.68486248	1.81789563	-7.02654351

H	-1.84538848	-0.34072891	-5.87822216
H	-3.56888887	1.35965968	-5.52761930
H	-1.03626303	7.76773779	-2.05413402
H	-0.09990057	6.01919816	-3.49214862
H	-2.50691029	6.08776062	-3.06296727
H	-5.78321104	4.21840147	3.17894427
H	-3.44583694	4.94588056	3.28954530
H	-4.74339207	5.31066462	1.24814355
Si	4.57901519	3.03992614	0.56659023
H	5.26027685	4.13001128	1.31856622
H	5.18027088	1.71727431	0.90287583
H	4.66408581	3.28244854	-0.90299326
Si	3.12545671	-2.08528365	-2.92412185
H	2.05855652	-2.63692753	-3.80927938
H	4.39097592	-1.89723326	-3.68652412
H	3.34419012	-2.98950184	-1.75853610

M_AlH$_3$·NMe$_3$_TS_HH (N/O *trans*) adduct

E: -1756.09539239 ; H: -1755.594170 ; G: -1755.754682

O	-2.25675848	0.52163165	2.74300850
Si	-1.71163680	0.81033365	1.23298148
O	-0.42718802	1.84590024	1.31340324
Si	0.98525604	2.27425164	0.58010113
O	2.03806310	2.79810588	1.70883883
O	-1.24580266	-0.60155012	0.53185582
Si	-1.09608618	-1.33274582	-0.93900935
O	-1.25935588	-2.94325406	-0.78724748
O	-2.91517610	1.51216496	0.34955810
Si	-3.15576820	2.57430010	-0.88866662
O	-1.95429498	3.70519120	-0.90308889
Si	-0.46781392	4.03387862	-1.53526352
O	-0.31385144	3.29812778	-3.00429936
Si	0.11996238	1.89150475	-3.74792962
O	1.29171745	1.15419620	-2.85683140
Si	1.59288579	0.12119748	-1.60983697
O	1.63161374	0.96971417	-0.19663614
O	0.41612116	-1.03054558	-1.53146745
O	-2.20775100	-0.71756339	-1.98113244
Si	-2.56344043	0.44026571	-3.09747909
O	-1.19500527	0.90272041	-3.89036917
O	3.03497564	-0.60310224	-1.84209654
O	-4.58476859	3.33335002	-0.66196121
O	-3.19112011	1.75595262	-2.31198765
O	0.69201125	3.47924345	-0.50450892
O	-0.31891218	5.64605520	-1.72318772
O	0.68807822	2.22900836	-5.23770865
Si	-5.04897781	4.94631154	-0.46144770
Si	0.30037768	6.67794477	-2.90942460
Si	0.28864773	1.76836647	-6.81410390
Si	-1.75629877	0.94343087	4.30027104
Si	-2.32907189	-4.19966646	-1.12686543
H	-1.50674540	-5.32520348	-1.65764209
H	-3.02710513	-4.60875082	0.12247870
H	-3.31516630	-3.77002320	-2.16577482
H	-2.58693623	0.14004507	5.24037691
H	-0.31006518	0.62091291	4.47187460
H	-1.98625335	2.40135987	4.51748800
H	1.18672028	2.54322913	-7.71550319
H	0.51945237	0.30406855	-6.97943464
H	-1.13929192	2.09991781	-7.08803131
H	0.41654923	8.02313548	-2.28133158
H	1.63736806	6.18837748	-3.35429918
H	-0.64201173	6.72004951	-4.06510667
H	-6.52988046	4.93186692	-0.29553486
H	-4.39409050	5.51051800	0.75389967
H	-4.66529939	5.73360099	-1.66861392

Si	3.57685409	2.34496477	2.23783263
H	3.94266569	3.29538310	3.32465782
H	3.53366637	0.94815162	2.76069137
H	4.54535599	2.44028187	1.10786599
Si	3.56970615	-2.20110009	-1.96537358
H	2.87450691	-2.87783639	-3.09860355
H	5.03597223	-2.13436745	-2.21784170
H	3.29045503	-2.92072784	-0.68870719
N	-6.75429501	-0.79170617	-0.37996276
C	-8.01281246	-0.84536206	-1.14851381
H	-8.43708288	-1.84841176	-1.08504802
H	-8.73414625	-0.12187317	-0.75201383
H	-7.81040937	-0.61090400	-2.19474052
C	-7.00816943	-1.13788363	1.03304514
H	-7.42005355	-2.14642294	1.09478032
H	-6.06956220	-1.10095300	1.58782844
H	-7.71744923	-0.43001690	1.47632669
C	-6.17115821	0.56339920	-0.46143551
H	-5.24342345	0.59028078	0.10991964
H	-5.96124868	0.80870712	-1.50315709
H	-6.86635706	1.30434278	-0.05278592
H	-6.22274321	-3.52351236	-1.07897562
H	-4.16763741	-1.95852806	-0.16340869
H	-5.25318119	-1.54542714	-2.65775132
Al	-5.40957659	-2.13933331	-1.16138148
H	-4.29255487	-0.71894279	-3.79457225
O	-3.62405026	-0.14516050	-4.19881714

M_AlH$_3$·NMe$_3$_TS_HH (N/O *trans*) TS

E: -1756.06602338 ; H: -1755.569357 ; G: -1755.726880

O	-1.03354030	0.71968407	3.48532721
Si	-0.82132169	0.91854463	1.88081113
O	0.43383332	1.96392153	1.62898851
Si	1.63682527	2.33192417	0.56516498
O	2.89738656	2.95967548	1.38560430
O	-0.46603231	-0.52881400	1.18019458
Si	-0.61793287	-1.39476962	-0.21444079
O	-0.73118987	-2.98395897	0.13104063
O	-2.20198566	1.53036635	1.22570870
Si	-2.73138375	2.47588382	-0.01470284
O	-1.59428167	3.62932115	-0.35693576
Si	-0.28428807	3.88780226	-1.32541422
O	-0.43734879	3.01229184	-2.71707414
Si	-0.09876554	1.56423566	-3.43202333
O	1.27680035	0.94369680	-2.77317762
Si	1.83551901	0.01256887	-1.53508317
O	2.12742595	0.96732816	-0.22347137
O	0.71873136	-1.14164420	-1.14884398
O	-1.97016627	-0.91620066	-1.02196636
Si	-2.55917503	0.16183860	-2.12409739
O	-1.36042691	0.52704401	-3.20617116
O	3.22420664	-0.71393141	-1.98369844
O	-4.11779586	3.22101352	0.42199424
O	-2.99358363	1.56007963	-1.35216640
O	1.08219102	3.43460409	-0.52701285
O	-0.19990155	5.47179866	-1.70447782
O	0.12997446	1.79353545	-5.03125714
Si	-4.63084233	4.82625529	0.50976983
Si	-0.21461481	6.36542523	-3.13702596
Si	-0.79104039	1.53112386	-6.42210675
Si	-0.09385176	0.96945156	4.86575724
Si	-1.96213768	-4.14009714	0.04055797
H	-1.43012840	-5.36509351	0.70025783
H	-3.17321417	-3.64339632	0.75574584
H	-2.28462109	-4.41457181	-1.38949976
H	-0.76700161	0.23875969	5.97526562

H	1.28087008	0.43140557	4.64420338
H	-0.02872400	2.42898594	5.16465359
H	-0.10628878	2.26001379	-7.52595647
H	-0.85012897	0.07063567	-6.71548392
H	-2.16917943	2.06941957	-6.22141924
H	-0.07318801	7.79461147	-2.74319136
H	0.92183759	5.94410429	-4.00625516
H	-1.50890711	6.14786437	-3.84843747
H	-6.08932465	4.78483270	0.81291518
H	-3.89196510	5.53526551	1.59399978
H	-4.39418753	5.50374910	-0.79910041
Si	4.56401957	2.69995737	1.45697881
H	5.12136363	3.78177667	2.31577588
H	4.83333370	1.36362373	2.06374798
H	5.14399976	2.76657742	0.08466193
Si	3.77210977	-2.30178017	-2.15651123
H	2.92644807	-3.02004798	-3.15329733
H	5.17910498	-2.20900027	-2.63708464
H	3.71516142	-2.99860749	-0.83884889
N	-7.72306575	-0.67548880	-1.64807690
C	-8.49337650	-0.76960714	-2.89906454
H	-8.34823333	-1.75529082	-3.34349863
H	-9.56163111	-0.61236492	-2.70841051
H	-8.14172483	-0.01284641	-3.60216670
C	-8.17539550	-1.71148591	-0.70299876
H	-8.01967637	-2.69801376	-1.14331165
H	-7.59910659	-1.63954143	0.22065925
H	-9.23997261	-1.58557458	-0.47346563
C	-7.89292963	0.65959179	-1.04893446
H	-7.29842666	0.72835173	-0.13687826
H	-7.54619349	1.41889411	-1.75180034
H	-8.94716168	0.84533467	-0.81178950
H	-5.86643424	-2.45165896	-2.72620673
H	-5.23261260	-0.77983422	-0.49512505
H	-5.82752652	0.38176032	-3.11150775
Al	-5.66577716	-1.04049848	-2.01098685
H	-4.82774458	0.18945685	-3.16726572
O	-3.84954420	-0.47640581	-2.89139050

M_AlH$_3$·NMe$_3$_TS_HH (N/O *trans*) product / H$_2$ adduct

E: -1756.13534361 ; H: -1755.638278 ; G: -1755.796444

O	-1.49297663	0.91989561	3.43098098
Si	-1.22405323	1.01550584	1.82535500
O	0.01514545	2.06955305	1.54311092
Si	1.24706586	2.40167131	0.49913180
O	2.46793792	3.09346770	1.32706438
O	-0.82539350	-0.47034399	1.23550040
Si	-0.93847333	-1.38818446	-0.13032380
O	-1.04703158	-2.96165041	0.28524655
O	-2.59672027	1.55052818	1.08669837
Si	-3.09223936	2.43907107	-0.21056664
O	-1.97090836	3.59617492	-0.57004843
Si	-0.64329361	3.82399033	-1.52610200
O	-0.75922198	2.87474250	-2.87008571
Si	-0.36789842	1.39678549	-3.49579381
O	1.00207273	0.85066305	-2.76198748
Si	1.53059443	-0.01577603	-1.46646925
O	1.78297678	1.00338927	-0.19551427
O	0.40953550	-1.15521882	-1.05207841
O	-2.27822311	-0.95403598	-0.98149021
Si	-2.84844678	0.01684882	-2.20157140
O	-1.60792396	0.34083276	-3.24698065
O	2.93176118	-0.76272563	-1.83844034
O	-4.51402794	3.15661813	0.15654334
O	-3.31443174	1.45133924	-1.50121840
O	0.70769164	3.42831131	-0.67123911

O	-0.57131804	5.38979385	-1.97201294
O	-0.09177499	1.54370321	-5.09639522
Si	-5.11474182	4.73446961	0.13853732
Si	-0.58170909	6.24726239	-3.42692787
Si	-0.99369978	1.26741724	-6.49844433
Si	-0.57989714	1.19344172	4.82583576
Si	-2.10819985	-4.22220149	-0.09464871
H	-1.59676440	-5.42446460	0.62157850
H	-3.48048539	-3.87789722	0.37855820
H	-2.11371471	-4.44943269	-1.56800536
H	-1.26684174	0.47057836	5.93219942
H	0.80279198	0.66492869	4.63501415
H	-0.53496798	2.65724083	5.10635954
H	-0.29215663	1.98499559	-7.59956494
H	-1.04289618	-0.19647049	-6.77658306
H	-2.37444614	1.80525294	-6.32261997
H	-0.49950862	7.68933290	-3.06513320
H	0.59156063	5.84501782	-4.25538336
H	-1.84889149	5.96462057	-4.16313986
H	-6.57827370	4.62648029	0.39785228
H	-4.45267845	5.53545706	1.20812420
H	-4.86734222	5.35304843	-1.19666477
Si	4.14563356	2.91852878	1.41124065
H	4.64440676	4.04542803	2.24735287
H	4.47563252	1.61100377	2.04959234
H	4.72750300	2.98231468	0.03960844
Si	3.46034912	-2.36678865	-1.88587140
H	2.72119377	-3.10481878	-2.95087176
H	4.91649947	-2.32072055	-2.19481443
H	3.22671305	-3.01116310	-0.56058466
N	-6.48280513	-0.74177986	-1.13385869
C	-6.72242088	0.67536837	-1.48346323
H	-7.30523947	0.72706490	-2.40442699
H	-7.26987975	1.17547197	-0.67719907
H	-5.76834367	1.17832899	-1.63474755
C	-7.77263349	-1.43295373	-0.93238753
H	-8.36541182	-1.37152830	-1.84621068
H	-7.59165034	-2.48288070	-0.69468402
H	-8.32731569	-0.96899198	-0.10972111
C	-5.68090890	-0.82464419	0.10461985
H	-5.47944518	-1.87055739	0.33896959
H	-4.73228176	-0.30691972	-0.02906176
H	-6.21779389	-0.35913811	0.93794567
H	-6.58124543	-1.55382771	-3.87612818
H	-5.19448716	-3.12462940	-2.05757418
H	-5.31400162	1.91816974	-4.54399288
Al	-5.52189356	-1.69099203	-2.68876320
H	-5.02991931	1.30875299	-4.21990446
O	-4.09666912	-0.65926030	-2.94414927

M_AlH$_3$·NMe$_3$_TS_HH (N/O *cis*) adduct

E: -1756.09691166 ; H: -1755.596067 ; G: -1755.754981

O	-1.55561846	0.68122997	2.97993710
Si	-1.09297685	0.95831727	1.44086012
O	0.21478397	1.96323540	1.42690700
Si	1.55798504	2.36221771	0.55649698
O	2.71478468	2.89175806	1.57351020
O	-0.70370157	-0.47437114	0.72245160
Si	-0.68677765	-1.20706823	-0.75342476
O	-0.93842310	-2.80557376	-0.56328832
O	-2.34904156	1.65161910	0.63028955
Si	-2.69091486	2.71607526	-0.57954804
O	-1.48062832	3.82361331	-0.70508509
Si	-0.04738948	4.12040904	-1.46288560
O	-0.04229605	3.36995839	-2.93437483
Si	0.33161846	1.95164572	-3.68608569

O	1.56349225	1.22411804	-2.87073657
Si	1.95349650	0.18759713	-1.65280150
O	2.11019553	1.02763577	-0.24538607
O	0.76127974	-0.94594931	-1.49253216
O	-1.89894410	-0.57582244	-1.67859144
Si	-2.31410259	0.55662050	-2.81104004
O	-0.99360723	0.96537281	-3.70491997
O	3.36112181	-0.55999074	-1.98723355
O	-4.09403514	3.46801504	-0.22259598
O	-2.85943197	1.89590774	-2.00198135
O	1.18012261	3.54114523	-0.52979544
O	0.13665962	5.72382723	-1.68160327
O	0.79160590	2.25486373	-5.21873705
Si	-5.34348363	4.19598520	-1.09669652
Si	0.34168682	6.75308206	-3.00663687
Si	0.26734678	1.79749339	-6.75962255
Si	-0.89474972	0.94331687	4.51471094
Si	-1.85422295	-3.96698765	-1.39025676
H	-1.40855575	-5.29126250	-0.87577161
H	-3.29960306	-3.74035230	-1.10361363
H	-1.59333590	-3.85507104	-2.85493041
H	-1.85206714	0.34391350	5.48547055
H	0.43495807	0.27296006	4.60623691
H	-0.75291725	2.40842954	4.75223869
H	1.21365546	2.42129091	-7.72524963
H	0.30115082	0.31107292	-6.87795328
H	-1.11921009	2.29946848	-6.98192880
H	0.66007591	8.09694939	-2.45026158
H	1.45956864	6.25695135	-3.86014139
H	-0.92428729	6.79835295	-3.79511275
H	-6.19237049	3.12792831	-1.70107691
H	-6.13154307	4.99941366	-0.12201732
H	-4.77193409	5.06779336	-2.16390768
Si	4.35005619	2.54909883	1.83259922
H	4.86656431	3.61739609	2.73202969
H	4.47553977	1.21167265	2.48141011
H	5.07812637	2.55823799	0.53054718
Si	3.83418654	-2.09583604	-2.50911031
H	3.07545572	-2.46130764	-3.74093665
H	5.29269299	-2.01252576	-2.79737984
H	3.56775585	-3.08976707	-1.42951775
H	-4.14300001	-0.55573432	-3.38452212
O	-3.45216617	-0.03358833	-3.82333083
H	-7.64155688	-1.30916564	-1.52668656
H	-6.06233006	-3.45049179	-0.81892286
H	-5.04264300	-1.41993982	-2.30490105
Al	-6.17679094	-1.91193241	-1.26301210
N	-5.59899282	-0.90842880	0.43437224
C	-6.53432140	-1.22403041	1.53182663
H	-6.25223259	-0.67970628	2.43981456
H	-7.54772119	-0.94111060	1.24283643
H	-6.50822010	-2.29599087	1.73323028
C	-5.62295449	0.54153040	0.15314399
H	-5.26757711	1.10746370	1.01943756
H	-4.97572884	0.75088964	-0.69920981
H	-6.64101375	0.84519845	-0.09369007
C	-4.22934888	-1.31545674	0.81156067
H	-3.55076562	-1.06003619	-0.00090688
H	-3.91593526	-0.79632076	1.72319327
H	-4.20339286	-2.39228660	0.98296075

M_AlH$_3$·NMe$_3$_TS_HH (N/O *cis*) TS

E: -1756.06662034 ; H: -1755.569772 ; G: -1755.725246

O	-0.71363201	0.75433670	3.52728454
Si	-0.53666710	0.94359501	1.91986095
O	0.73463678	1.95323743	1.62051734

Si	1.91466090	2.29856826	0.52185701
O	3.22080179	2.87900037	1.30074017
O	-0.25570930	-0.51729180	1.21179296
Si	-0.48680057	-1.34531225	-0.19257641
O	-0.69185927	-2.92960479	0.11477848
O	-1.92004080	1.58938397	1.29398991
Si	-2.46108853	2.60129876	0.11672318
O	-1.30965676	3.71575462	-0.26715432
Si	-0.02595691	3.93246348	-1.28390810
O	-0.27067008	3.05835915	-2.66504927
Si	0.01686764	1.62588871	-3.42650305
O	1.37622334	0.93908058	-2.80924982
Si	1.96415670	-0.01230905	-1.59661964
O	2.33369255	0.92637018	-0.29596408
O	0.81740614	-1.12607133	-1.17656839
O	-1.84052852	-0.76883872	-0.94519534
Si	-2.41488522	0.33040344	-2.02570047
O	-1.28605030	0.62644336	-3.18447740
O	3.30887406	-0.78092827	-2.09732095
O	-3.81958886	3.33107132	0.63992717
O	-2.81247512	1.71849622	-1.23801743
O	1.35046428	3.42447087	-0.54078362
O	0.09639159	5.51048800	-1.66655949
O	0.20388232	1.87166913	-5.02456657
Si	-4.84985399	4.57561824	0.14658817
Si	0.10299302	6.40960044	-3.09804315
Si	-0.73847086	1.63985876	-6.41045578
Si	0.24423744	1.00938472	4.89690336
Si	-1.88651094	-4.07000974	-0.27461846
H	-1.28374097	-5.40555169	-0.00572756
H	-3.07274671	-3.84417982	0.59981769
H	-2.25908271	-3.92753423	-1.71008404
H	-0.41764659	0.28276168	6.01514643
H	1.61433101	0.46896641	4.65592013
H	0.31197318	2.47047433	5.18549659
H	-0.04872523	2.36399960	-7.51329285
H	-0.82627288	0.18208377	-6.70807258
H	-2.10127020	2.20389279	-6.18301448
H	0.30245591	7.83041763	-2.70113240
H	1.21479950	5.94323376	-3.97608971
H	-1.20539629	6.24001797	-3.79572700
H	-5.52402894	4.17215976	-1.12306369
H	-5.85087220	4.75289144	1.23396617
H	-4.05956752	5.82209008	-0.06340342
Si	4.87127940	2.51864016	1.36366172
H	5.49116890	3.55240534	2.23796436
H	5.05904095	1.15802103	1.94550282
H	5.44767720	2.57473574	-0.01029550
Si	3.69719362	-2.33057795	-2.65148510
H	2.75538862	-2.72098747	-3.74096340
H	5.09185671	-2.25507654	-3.16707337
H	3.60425282	-3.29666715	-1.51983106
H	-3.76255763	-1.05832364	-3.44347589
O	-3.79386295	-0.26111496	-2.71329004
H	-6.70630137	-1.28367013	-3.22735314
H	-5.09714163	-2.91016260	-1.48972618
H	-4.31486265	-2.07253830	-3.81581502
Al	-5.35873426	-1.64092438	-2.43620611
N	-5.98523116	-0.44546498	-0.73213641
C	-7.26248056	-1.05829344	-0.32575075
H	-7.67041854	-0.54703075	0.55431005
H	-7.97995722	-0.99207632	-1.14433497
H	-7.10062792	-2.11044626	-0.08339884
C	-6.21511792	0.96202704	-1.10052841
H	-6.65790852	1.51057501	-0.25982006
H	-5.27154764	1.42916764	-1.37630445
H	-6.89521555	1.00479255	-1.95301277

C	-5.04425142	-0.53016405	0.39705413
H	-4.09851076	-0.05897224	0.14118245
H	-5.45161106	-0.02410965	1.28046431
H	-4.85759391	-1.57812742	0.63419608

M_AlH_3·NMe_3_TS_HH (N/O *cis*) product / H_2 adduct

E: -1756.13487448 ; H: -1755.637048 ; G: -1755.797817

O	-0.69681689	0.78428803	3.55210716
Si	-0.54160794	0.96929739	1.93947874
O	0.73556313	1.96996239	1.62979716
Si	1.90947215	2.30415810	0.52148799
O	3.22709003	2.87401446	1.29206833
O	-0.27881976	-0.49562262	1.23545726
Si	-0.54043781	-1.31141553	-0.17398576
O	-0.73405653	-2.89948025	0.14712345
O	-1.92642436	1.62931863	1.33601635
Si	-2.45820225	2.62833572	0.13910021
O	-1.30203959	3.74490707	-0.23348749
Si	-0.03208967	3.95004022	-1.26789436
O	-0.29660009	3.08424027	-2.64850758
Si	-0.04018761	1.63729515	-3.39772827
O	1.33580029	0.95932614	-2.79875606
Si	1.91573719	-0.00353800	-1.59412128
O	2.31477576	0.92676298	-0.29441038
O	0.76335230	-1.10596742	-1.16437018
O	-1.89843515	-0.73704473	-0.89974296
Si	-2.50292376	0.33462974	-2.01521632
O	-1.32965096	0.64113118	-3.14062159
O	3.24829860	-0.79070362	-2.10533256
O	-3.80770086	3.37664818	0.67589353
O	-2.81988350	1.75121004	-1.20270021
O	1.35064652	3.43475344	-0.53821761
O	0.10036683	5.52926031	-1.65016419
O	0.13674539	1.88156100	-5.00107759
Si	-4.80643192	4.64753570	0.19476140
Si	0.11158814	6.41937845	-3.08597507
Si	-0.81384225	1.59904529	-6.36889706
Si	0.27501477	1.08288337	4.90119621
Si	-1.87934356	-4.05751571	-0.31043048
H	-1.31997876	-5.37774205	0.09487946
H	-3.16054077	-3.79553471	0.40801181
H	-2.09354907	-4.00244818	-1.78467370
H	-0.36071597	0.37046103	6.04416638
H	1.65067596	0.55877604	4.65618999
H	0.32508848	2.55014726	5.16303251
H	-0.14471186	2.30442012	-7.49744158
H	-0.88234194	0.13358916	-6.63634364
H	-2.18481256	2.14639429	-6.15058106
H	0.32412398	7.84110956	-2.69754321
H	1.21759873	5.94181657	-3.96557692
H	-1.19925121	6.26026154	-3.78182297
H	-5.51127730	4.26307605	-1.06486803
H	-5.79225696	4.85302748	1.29215971
H	-3.99217425	5.87634524	-0.02766776
Si	4.87015872	2.48409172	1.34459916
H	5.51406803	3.50302714	2.21957926
H	5.03922726	1.11844487	1.92074775
H	5.44253052	2.53556608	-0.03134005
Si	3.60843798	-2.35321869	-2.63627212
H	2.65426256	-2.75049948	-3.71277711
H	5.00024539	-2.30826314	-3.16394244
H	3.51205208	-3.30253089	-1.49021119
H	-3.41138277	-2.13382472	-4.60334433
O	-3.84792210	-0.23178745	-2.67624142
H	-6.43054763	-1.08883852	-3.35834072
H	-4.86892086	-2.73259192	-1.75916320

H	-3.73114068	-2.78951661	-4.75926116
Al	-5.24068688	-1.27736088	-2.30963803
N	-6.01621306	-0.38598717	-0.61711022
C	-7.28935113	-1.06863933	-0.31059396
H	-7.74789633	-0.63383715	0.58433898
H	-7.97473499	-0.96307874	-1.15282915
H	-7.10103575	-2.12952189	-0.13485613
C	-6.26405165	1.04778520	-0.87885805
H	-6.71488973	1.51910569	0.00153651
H	-5.32085726	1.53954826	-1.11361252
H	-6.94084003	1.14953491	-1.72867332
C	-5.09358888	-0.53487325	0.52776936
H	-4.15431540	-0.02436161	0.32212459
H	-5.53661770	-0.10120095	1.43065459
H	-4.88784784	-1.59273031	0.69485017

M_$AlH_2 \cdot NMe_3$

E: -1754.95718644 ; H: -1754.475668 ; G: -1754.628472

O	-1.05799233	0.88348183	3.49906927
Si	-0.83555286	1.07317810	1.89481176
O	0.48504545	2.03365141	1.63964449
Si	1.70197815	2.31255379	0.56185652
O	3.02758081	2.82200343	1.36239225
O	-0.59255561	-0.39341162	1.18739665
Si	-0.85588932	-1.20299719	-0.22656918
O	-1.12027658	-2.78297644	0.08761986
O	-2.17426049	1.78115943	1.24416259
Si	-2.63371198	2.80295652	0.03443398
O	-1.42430150	3.87952276	-0.29101602
Si	-0.11485610	4.03905632	-1.28395125
O	-0.36906724	3.18890808	-2.67495663
Si	-0.14040881	1.73386716	-3.41887575
O	1.19462790	1.00982643	-2.77954946
Si	1.68450963	0.01148506	-1.56558758
O	2.06272268	0.91481372	-0.23935204
O	0.47743972	-1.05094814	-1.18511265
O	-2.17739528	-0.57827541	-0.98020919
Si	-2.69683885	0.51345955	-2.11821923
O	-1.46599886	0.78075926	-3.19111967
O	3.00026463	-0.82546508	-2.03985630
O	-3.96630811	3.61998254	0.51343872
O	-2.99378239	1.93949672	-1.31291088
O	1.22191308	3.46514834	-0.51207587
O	-4.02921808	0.00454719	-2.84584803
O	0.09236231	5.61414440	-1.64745934
O	0.08963040	1.97380813	-5.01535340
Si	-4.42119070	5.24548803	0.56221386
Si	0.23547109	6.51634578	-3.06877314
Si	-0.82808534	1.72151929	-6.41164776
Si	-0.12049399	1.11828544	4.88472494
Si	-2.45180300	-3.80160163	-0.14250474
H	-2.08332536	-5.11046969	0.46724724
H	-3.64372864	-3.22645497	0.54769924
H	-2.72528045	-3.95388756	-1.59923363
H	-0.81366652	0.40116719	5.99089049
H	1.24451450	0.55383880	4.67052208
H	-0.03211274	2.57687282	5.18132600
H	-0.12196686	2.43446789	-7.51274941
H	-0.90611667	0.26081014	-6.69979305
H	-2.19721558	2.28357679	-6.22125274
H	0.55230198	7.91052921	-2.65198377
H	1.33099854	5.95776334	-3.91270053
H	-1.05663660	6.47505127	-3.81403770
H	-5.88342172	5.26024842	0.84982205
H	-3.66892190	5.94561171	1.64261039
H	-4.14592739	5.88587892	-0.75716556

Si	4.63285815	2.30727750	1.47747323
H	5.35726627	3.35533945	2.24892801
H	4.68384008	1.00127708	2.19725850
H	5.21598438	2.16331231	0.11207714
Si	3.44476474	-2.45468515	-2.08071232
H	2.67297048	-3.15572406	-3.14719898
H	4.90252399	-2.48571440	-2.38423339
H	3.17374039	-3.08291915	-0.75477275
H	-6.60514193	-0.64474552	-3.73597381
H	-5.33024036	-2.37048136	-1.97778600
Al	-5.53531467	-0.90030583	-2.57736522
N	-6.37749478	0.09258064	-0.98210579
C	-7.72554434	-0.47913902	-0.78791215
H	-7.64197041	-1.54811177	-0.58303075
H	-8.22844978	0.00948930	0.05355469
H	-8.31547778	-0.33432971	-1.69409173
C	-5.57589966	-0.10648858	0.24330563
H	-5.47311817	-1.17359298	0.44336419
H	-4.58403369	0.32410133	0.11295721
H	-6.05866278	0.38155309	1.09674692
C	-6.48259710	1.53624641	-1.28453459
H	-5.48562168	1.95114075	-1.42766363
H	-7.06254088	1.67261897	-2.19862300
H	-6.97638062	2.05984182	-0.45876409

Bipodal site B^0

B^0

E: -1572.64333315 ; H: -1572.316896 ; G: -1572.452007

O	-0.36734580	0.84129126	4.05598538
Si	-0.51173892	0.99856910	2.44029620
O	0.55924788	2.12419670	1.89062723
Si	1.43073898	2.54276100	0.55893004
O	2.77671891	3.32173605	1.04483760
O	-0.20028272	-0.44884747	1.71028065
Si	-0.60385482	-1.37519534	0.40920139
O	-0.48237082	-2.95177805	0.80352258
O	-2.04932696	1.47817426	2.10162921
Si	-2.96240191	2.30434866	1.00256213
O	-2.04693267	3.52285800	0.36871123
Si	-1.01833293	3.85664925	-0.87381635
O	-1.40478213	2.92592454	-2.18261380
Si	-1.09495682	1.48393480	-2.91367017
O	0.44972025	1.01848637	-2.57635553
Si	1.34189333	0.17222131	-1.48241678
O	1.84663701	1.18630365	-0.28645729
O	0.42476051	-1.04115000	-0.83308988
O	-2.15791582	-1.04380514	-0.04599642
Si	-3.04358332	-0.06016222	-1.03574119
O	-2.14646952	0.33966921	-2.35482267
O	2.63654454	-0.48335681	-2.22473934
O	-4.32549980	2.89179076	1.70471931
O	-3.46858459	1.29087689	-0.19043604
O	0.52795387	3.52714375	-0.40825725
O	-4.37740519	-0.83541045	-1.59736364
O	-1.15257340	5.42995890	-1.27538015
O	-1.27504389	1.65163068	-4.52341774
H	-4.20063037	3.53616284	2.40272112
H	-5.08475638	-0.97608302	-0.96670990
Si	-1.16997135	6.31241787	-2.71681581
Si	-2.10457425	0.86625812	-5.76777878
Si	0.64419995	0.01722152	5.12768611
Si	-1.53379722	-4.27045377	0.89130491
H	-0.71969822	-5.42803048	1.35390551
H	-2.62411328	-3.97428096	1.86696466
H	-2.11503965	-4.53935274	-0.45567989
H	0.64972509	0.79139210	6.40002862

H	0.09852715	-1.35251381	5.35411092
H	2.02089338	-0.06692476	4.55776206
H	-1.59805364	1.44778294	-7.04146800
H	-1.82439575	-0.59819140	-5.71344833
H	-3.56813275	1.11418841	-5.62234815
H	-1.03270138	7.74514627	-2.33536328
H	-0.02856681	5.88607857	-3.57812837
H	-2.46185723	6.07950091	-3.42491893
Si	4.23126195	3.81897230	0.34450507
H	4.66437994	5.04669277	1.06798154
H	5.24132938	2.73414031	0.50448751
H	4.01574320	4.11180521	-1.10338396
Si	3.32336051	-2.02532741	-2.30578360
H	2.36472831	-2.96508282	-2.95623960
H	4.56182127	-1.89179187	-3.12149428
H	3.65120790	-2.49934074	-0.92965187

B^{0}_AlH_3·NMe_3_TS_HH (N/O *trans*) adduct

E: -1750.97413535 ; H: -1750.491099 ; G: -1750.641381

O	-2.00453017	-0.03388507	3.90485130
Si	-1.82720316	0.35676188	2.33745839
O	-1.01538440	1.78866755	2.18815716
Si	0.00986607	2.61807868	1.21185437
O	0.91434368	3.62875713	2.12096549
O	-0.92097072	-0.82417324	1.62078662
Si	-0.75286068	-1.57888528	0.17025548
O	-0.30291816	-3.12812549	0.40986420
O	-3.27747562	0.43244304	1.56402853
Si	-4.12348995	1.23539738	0.39862902
O	-3.41574335	2.70723032	0.13657516
Si	-2.26543765	3.49465533	-0.73170292
O	-2.03950281	2.75823190	-2.18940982
Si	-1.19207654	1.54197377	-2.91561219
O	0.28580797	1.42439931	-2.20047934
Si	1.09007989	0.66579529	-0.97978288
O	1.00689298	1.58361858	0.39501924
O	0.40813161	-0.80669283	-0.71141757
O	-2.18156893	-1.55276496	-0.66004387
Si	-3.05324900	-0.69901035	-1.77259582
O	-2.01853433	0.12354930	-2.75496128
O	2.65301142	0.48827722	-1.40394736
O	-4.06732828	0.33902457	-0.98778541
O	-0.85948051	3.50775061	0.12748984
O	-3.90753160	-1.70605456	-2.75051219
O	-2.74416728	5.03626769	-0.98475465
O	-1.00820659	1.88731144	-4.49671014
H	-4.68574738	-2.10967057	-2.36407651
Si	-2.96924035	6.02712515	-2.33422018
Si	-1.59003177	1.27083424	-5.95837280
Si	-2.96320798	0.25224485	5.26065619
Si	-0.84409962	-4.64724709	-0.08617110
H	0.10720645	-5.64189179	0.48172764
H	-2.22157772	-4.88288483	0.43761669
H	-0.84972333	-4.71858743	-1.57654627
H	-2.56063871	1.53284260	5.90872597
H	-4.40565367	0.28386624	4.88417344
H	-2.70095145	-0.88833500	6.18685933
H	-1.07562046	2.17335394	-7.02553387
H	-1.08131937	-0.11704890	-6.15358876
H	-3.08185338	1.27471558	-5.94488851
H	-3.40199554	7.35187548	-1.80583443
H	-1.68564362	6.15750031	-3.08220680
H	-4.02513771	5.44870662	-3.21401729
Si	2.54928422	4.04034404	2.21452674
H	2.65037454	5.12535288	3.22987907
H	3.34415371	2.85026368	2.63679836

H	3.02342278	4.52183116	0.88382760
Si	4.17333504	0.73990898	-0.71888528
H	4.38847666	-0.22966151	0.39458625
H	5.17053921	0.52277978	-1.80288514
H	4.26175976	2.13678954	-0.19871088
H	-5.86540630	2.10116455	1.46917173
O	-5.69932493	1.42261756	0.79772987
H	-5.88331161	3.40474675	2.63052061
H	-3.49140894	2.49323529	3.49139163
H	-5.30738664	3.48735275	5.29520808
Al	-4.75056515	3.42981507	3.79119084
N	-3.90956584	5.28452131	3.55122603
C	-2.83725415	5.43736446	4.55701812
H	-2.35733380	6.41660393	4.45285612
H	-3.25993102	5.34648984	5.55869814
H	-2.08959598	4.65554131	4.41203437
C	-3.33207833	5.38759196	2.19508876
H	-2.58085242	4.60851937	2.06829698
H	-4.11376702	5.25133438	1.44849762
H	-2.86199605	6.36654555	2.05253691
C	-4.93494739	6.32945360	3.74271048
H	-5.71719109	6.21233651	2.99121331
H	-5.37677065	6.23072277	4.73538626
H	-4.48758988	7.32449890	3.64266333

B^{0}_AlH_3·NMe_3_TS_HH (N/O *trans*) TS

E: -1750.94275496 ; H: -1750.465671 ; G: -1750.616236

O	-0.85973829	0.90205715	4.02219256
Si	-0.93259492	1.03107520	2.39817082
O	-0.01278280	2.31075186	1.91965445
Si	0.89749024	2.85926994	0.66202688
O	2.08743563	3.82137856	1.22506425
O	-0.34122786	-0.36394095	1.72723659
Si	-0.53799124	-1.30626304	0.39113038
O	-0.24140900	-2.86016143	0.78946210
O	-2.48294743	1.23473503	1.89964998
Si	-3.43986807	1.99741737	0.79137951
O	-2.65030602	3.31891387	0.18203223
Si	-1.58669069	3.81233286	-0.96596069
O	-1.71731607	2.86202773	-2.31292618
Si	-1.15637561	1.46726608	-2.98761052
O	0.40540946	1.22525334	-2.52368807
Si	1.31376167	0.50499883	-1.35501848
O	1.57649236	1.57487088	-0.12906187
O	0.52476524	-0.82539005	-0.77442533
O	-2.08114630	-1.17590088	-0.18218882
Si	-3.02401342	-0.32676885	-1.24293759
O	-2.09138006	0.19814482	-2.49449763
O	2.74368536	0.04152091	-1.98729907
O	-3.72185208	0.93943354	-0.45300649
O	-0.04893795	3.71334811	-0.37856629
O	-4.17460274	-1.29720606	-1.90437953
O	-1.91823592	5.35627808	-1.37942747
O	-1.22147089	1.58512344	-4.61180453
H	-4.91779529	-1.51102697	-1.33884357
Si	-1.92196881	6.23978311	-2.81783468
Si	-2.13139854	0.89802473	-5.85719853
Si	-0.68453751	-0.36282144	5.12472173
Si	-0.97101096	-4.35302027	0.49201167
H	-0.04678831	-5.38864130	1.03149221
H	-2.28737073	-4.41386581	1.19213745
H	-1.16435815	-4.53668504	-0.97623295
H	-0.86312969	0.22696455	6.48093533
H	-1.72404749	-1.40323576	4.86851950
H	0.67653710	-0.95922127	4.99165458
H	-1.70914996	1.58382370	-7.11041045

H	-1.84736599	-0.56373445	-5.93966974
H	-3.58373974	1.12529547	-5.60162509
H	-1.98362213	7.67751915	-2.43261604
H	-0.67652837	5.95765940	-3.58966586
H	-3.11994217	5.86804359	-3.62574182
Si	3.77280200	3.75633087	1.29191240
H	4.21211896	4.97326225	2.02985814
H	4.20014060	2.52405361	2.01733530
H	4.32976247	3.75330179	-0.09169935
Si	3.66763861	-1.37142514	-1.97481632
H	2.95596997	-2.44206226	-2.73162925
H	4.95983068	-1.03746735	-2.63590924
H	3.89805203	-1.80841208	-0.56659475
H	-5.32260559	3.57004499	1.32934154
O	-4.83882761	2.46339161	1.48715405
H	-5.66795993	4.45633921	1.69064841
H	-3.48140563	3.84002974	3.49481469
H	-6.10748331	2.80133158	3.98552494
Al	-5.03933884	3.67651445	3.18864097
N	-5.57543638	5.52496458	4.09412041
C	-5.25268109	5.39590278	5.52564704
H	-5.49665361	6.32026010	6.06248573
H	-5.82381379	4.57108992	5.95511140
H	-4.18776519	5.18727486	5.64169765
C	-4.79203548	6.62212659	3.50193480
H	-3.72793758	6.41081086	3.61491072
H	-5.02207815	6.70380860	2.43837327
H	-5.02570776	7.57368801	3.99422986
C	-7.01519635	5.78138641	3.92618119
H	-7.24668473	5.87289638	2.86383694
H	-7.58314564	4.94734069	4.34085119
H	-7.30618591	6.70684697	4.43730334

B^{0}_AlH_3·NMe_3_TS_HH (N/O *trans*) product / H_2 adduct

E: -1751.01278486 ; H: -1750.534295 ; G: -1750.687260

O	-0.82214642	0.91761927	4.17997383
Si	-0.97681646	1.07260021	2.56442262
O	-0.18556032	2.44016107	2.09245626
Si	0.65840310	3.09162707	0.83360517
O	1.81342414	4.08857560	1.40872043
O	-0.31514340	-0.23584175	1.80531554
Si	-0.52124051	-1.13977701	0.44397121
O	-0.10562861	-2.68287963	0.76569790
O	-2.56908827	1.17577634	2.16543259
Si	-3.62661633	1.91389643	1.12271787
O	-2.86796334	3.27381028	0.54321670
Si	-1.93850754	3.93981905	-0.63268489
O	-2.07974455	3.06920586	-2.02955539
Si	-1.47855593	1.72978366	-2.78079470
O	0.11619220	1.57090171	-2.39591072
Si	1.12145495	0.85693236	-1.30627024
O	1.37157262	1.88571668	-0.04127078
O	0.44751907	-0.54526116	-0.75227457
O	-2.09515110	-1.08621451	-0.05096020
Si	-3.14509560	-0.26803310	-1.03168890
O	-2.30479020	0.39018472	-2.28610088
O	2.54565775	0.51796831	-2.02307738
O	-3.90959079	0.89437857	-0.15041628
O	-0.36973549	3.95237895	-0.12416182
O	-4.24048518	-1.29343986	-1.70260080
O	-2.42733307	5.47212954	-0.91007563
O	-1.63604185	1.90400456	-4.39220083
H	-4.96864506	-1.55815265	-1.13913757
Si	-3.05483414	6.32117940	-2.22871458
Si	-2.43489737	1.10215726	-5.64589642
Si	-1.78792031	0.43815104	5.47978155

Si	-0.65323267	-4.21431626	0.31286994
H	0.32596448	-5.19274617	0.86111024
H	-2.00822028	-4.44962368	0.89149271
H	-0.71055198	-4.30676713	-1.17539051
H	-2.39133767	1.65491310	6.09744129
H	-2.85679360	-0.48869504	5.01069701
H	-0.89084566	-0.24159568	6.45683907
H	-2.10042076	1.84145423	-6.89491707
H	-1.95231561	-0.30695478	-5.72719407
H	-3.90552026	1.12838908	-5.39904048
H	-3.24162503	7.72546833	-1.76730168
H	-2.09282169	6.26671881	-3.36689884
H	-4.36333423	5.72739350	-2.62955687
Si	3.50019688	4.06195607	1.50237882
H	3.89594227	5.27563041	2.26965640
H	3.94336808	2.82705592	2.21320958
H	4.07720639	4.09843463	0.12792367
Si	3.58150129	-0.81493747	-2.08567750
H	2.90787585	-1.93937048	-2.79746151
H	4.79186729	-0.37271965	-2.83220342
H	3.94442543	-1.23172468	-0.69953380
H	-5.86695142	3.88713722	0.02150585
O	-4.98213268	2.33104245	1.87282602
H	-6.08535857	4.35720219	-0.51530907
H	-4.94855401	2.06401858	4.70347198
H	-7.00143802	3.45386823	3.45606259
Al	-5.49331880	2.92741364	3.47068335
N	-4.41864941	4.67150199	3.68549416
C	-4.91322749	5.31604937	4.91929640
H	-4.38183011	6.25721095	5.09678456
H	-5.98089199	5.51872388	4.82280120
H	-4.75063690	4.64888516	5.76803164
C	-2.97223793	4.39608104	3.82304922
H	-2.81106221	3.68586773	4.63491501
H	-2.58350831	3.98177348	2.89378371
H	-2.43140413	5.32327752	4.04112583
C	-4.65164430	5.55724070	2.52477139
H	-4.26825899	5.08030870	1.62350951
H	-5.72231101	5.73387001	2.41051800
H	-4.14029725	6.51526880	2.66981459

B^{0}_AlH_3·NMe_3_TS_HH (N/O *cis*) adduct

E: -1750.97670965 ; H: -1750.493834 ; G: -1750.645426

O	-0.74533208	1.37750803	3.50986223
Si	-0.80724937	1.27097317	1.88300929
O	0.70251251	1.51103116	1.26031270
Si	1.49778408	2.05738483	-0.08552345
O	2.94988853	2.64344664	0.36537896
O	-1.34110923	-0.23384575	1.46301968
Si	-1.22537783	-1.38918572	0.29540240
O	-1.44089074	-2.85446467	0.98344781
O	-1.85404006	2.40161405	1.31286232
Si	-2.88734192	2.71607150	0.05825184
O	-2.05942851	3.46114794	-1.15322043
Si	-0.58770896	3.50336286	-1.89937182
O	-0.51778190	2.32935820	-3.05359663
Si	-1.03032504	0.82413098	-3.49751737
O	0.00472524	-0.31189909	-2.90134644
Si	1.05799570	-0.60114862	-1.66285879
O	1.71337737	0.82117895	-1.14990621
O	0.26019277	-1.31197439	-0.40858409
O	-2.40602601	-1.15735833	-0.83409396
Si	-3.31649859	0.02798256	-1.54620765
O	-2.54146326	0.54958731	-2.90202922
O	2.23878166	-1.59479140	-2.18453353
O	-3.48544798	1.26794349	-0.46941636

O	0.60696036	3.24647992	-0.79517097
O	-0.38179251	4.96170265	-2.59514100
O	-1.05425828	0.72967154	-5.12399495
Si	-1.30960357	6.35415180	-2.82879406
Si	-0.81851701	1.80636157	-6.40447624
Si	0.45004393	1.36803291	4.70203800
Si	-2.39902296	-4.20103896	0.63984237
H	-1.97177912	-5.27560566	1.57760703
H	-3.83240766	-3.85155100	0.87222324
H	-2.20309743	-4.62350932	-0.77648971
H	1.39282261	2.50161516	4.47257682
H	-0.25294598	1.52390530	6.00521198
H	1.19112460	0.07332705	4.65794345
H	0.60369633	2.25626299	-6.41955510
H	-1.14299604	1.05667171	-7.64912326
H	-1.72527887	2.98082294	-6.24728169
H	-1.82510472	6.84275176	-1.51765660
H	-0.40174689	7.36235173	-3.44356395
H	-2.44430394	6.04489329	-3.74691316
Si	3.68961268	3.07844530	1.81964596
H	2.85838537	4.10318929	2.51713130
H	3.83309880	1.87122564	2.68539265
H	5.02511916	3.63382531	1.46786206
Si	2.76401365	-2.17747034	-3.68136064
H	1.72845571	-3.08660260	-4.25118701
H	3.00862773	-1.03330989	-4.60741100
H	4.02801636	-2.92094984	-3.42180288
H	-5.52185200	-0.14310125	-1.44876440
O	-4.79216393	-0.57679532	-1.91916838
H	-4.84699260	3.26945289	0.95255973
O	-4.10111586	3.70926415	0.51764643
H	-6.49908647	0.63921269	-0.40491158
H	-8.34385022	0.88328649	1.55621212
H	-6.00356318	2.28114110	1.70529788
Al	-6.80469854	1.00280421	1.13037854
N	-5.93328527	-0.54032530	2.18257990
C	-6.15011684	-1.80272894	1.44364168
H	-5.63179933	-1.75703680	0.48525809
H	-5.76718075	-2.65060498	2.02142787
H	-7.21751082	-1.94622814	1.26490338
C	-6.57488803	-0.62431353	3.51246320
H	-6.44734601	0.32387591	4.03800171
H	-7.63986157	-0.82337659	3.39460311
H	-6.11449278	-1.42499182	4.10130993
C	-4.48207252	-0.31363082	2.35606345
H	-4.00575972	-0.21515356	1.38351441
H	-4.32186639	0.60636223	2.91888059
H	-4.02940088	-1.15148656	2.89623841

B^{0}_AlH_3·NMe_3_TS_HH (N/O *cis*) TS

E: -1750.94547766 ; H: -1750.466783 ; G: -1750.614298

O	-0.32202132	1.27113222	3.62770889
Si	-0.62303207	1.24794941	2.02508488
O	0.78649822	1.51371189	1.20549109
Si	1.50181631	2.08919431	-0.17026776
O	2.98068374	2.66610628	0.19374424
O	-1.22448003	-0.23090196	1.59641747
Si	-1.15879897	-1.40299152	0.43713458
O	-1.16442141	-2.87499412	1.13492179
O	-1.73233071	2.41217478	1.67686706
Si	-2.78419574	2.74137941	0.44334932
O	-2.04832575	3.76908660	-0.62112888
Si	-0.78577021	3.58765346	-1.67658295
O	-1.06983256	2.32123924	-2.68756797
Si	-1.37039170	0.84789553	-3.34989134
O	-0.18291483	-0.21202094	-2.92349742

Si	0.93589468	-0.53352527	-1.75180056
O	1.64589954	0.86885617	-1.26645811
O	0.20621708	-1.24317566	-0.45545604
O	-2.50394167	-1.26350129	-0.52748697
Si	-3.32446767	-0.02164262	-1.23591157
O	-2.80743156	0.25271689	-2.77162174
O	2.06101220	-1.54166546	-2.35856658
O	-3.07224749	1.32385609	-0.33984165
O	0.59013259	3.29655615	-0.81753780
O	-0.62013432	4.94507932	-2.55769732
O	-1.45815147	0.97071128	-4.96992241
Si	-1.17487241	6.54040653	-2.52867080
Si	-1.30956622	2.23566683	-6.08515754
Si	1.04073234	1.08317143	4.60689952
Si	-2.15070432	-3.77305186	2.16653554
H	-1.26126031	-4.62555023	3.00165021
H	-2.94571689	-2.84422548	3.02563144
H	-3.07281441	-4.61055954	1.34632078
H	2.00288633	2.19147280	4.33867002
H	0.56268144	1.13363538	6.01617065
H	1.68577376	-0.23124707	4.31631568
H	0.04092121	2.85501231	-5.95393952
H	-1.48135752	1.62709046	-7.43282154
H	-2.36976614	3.25205677	-5.82487861
H	-0.88615946	7.14712397	-1.19698723
H	-0.43502654	7.25872332	-3.60324243
H	-2.64126086	6.55968297	-2.79769405
Si	3.94882485	2.83298968	1.56594143
H	3.37061031	3.88178137	2.45600931
H	4.01331352	1.53099521	2.29258371
H	5.29974086	3.23763930	1.08868486
Si	2.38619902	-2.24224432	-3.86219786
H	1.21512390	-3.05551568	-4.29894655
H	2.66753534	-1.16936149	-4.86014419
H	3.58383426	-3.10624057	-3.67141576
H	-5.58507273	0.24642506	-1.85939721
O	-4.94112804	-0.37973378	-1.23598844
H	-4.97341366	2.89753639	0.81447140
O	-4.16611416	3.39242209	1.02504130
H	-6.56092210	0.94336509	-1.86845184
H	-7.94091394	-0.41027193	-0.18673776
H	-6.27153964	1.81103527	0.55286609
Al	-6.56314522	0.39856218	-0.17463591
N	-5.89580894	-0.70544808	1.56644724
C	-5.70283421	-2.12878906	1.23593218
H	-4.86154560	-2.23598283	0.55166783
H	-5.51117351	-2.71203352	2.14421347
H	-6.60136543	-2.51264566	0.74971687
C	-7.00514958	-0.57262049	2.53012682
H	-7.17744727	0.48411446	2.74555133
H	-7.91420375	-0.99922633	2.10694593
H	-6.76157648	-1.09068227	3.46505014
C	-4.67426615	-0.16225700	2.18490616
H	-3.82589033	-0.28543362	1.51721349
H	-4.81193305	0.89902266	2.39402820
H	-4.45203807	-0.68235585	3.12376838

B^{0}_AlH_3·NMe_3_TS_HH (N/O *cis*) product / H_2 adduct

E: -1751.01332645 ; H: -1750.533378 ; G: -1750.684052

O	-0.16241755	1.09870271	3.66131696
Si	-0.50956864	1.11031368	2.06585684
O	0.88121558	1.40391147	1.22129641
Si	1.55532096	1.99597148	-0.16869265
O	3.03933761	2.58249479	0.16381698
O	-1.12589090	-0.35778611	1.63306754
Si	-1.08435894	-1.50443305	0.44187026

O	-1.06040686	-2.98679401	1.13012784
O	-1.62217613	2.28955359	1.77004233
Si	-2.70403588	2.60065828	0.55749027
O	-2.02005815	3.66781697	-0.50752428
Si	-0.78428937	3.49955412	-1.59761165
O	-1.08666024	2.25517616	-2.62754833
Si	-1.40374870	0.77541971	-3.27835144
O	-0.18259977	-0.26787979	-2.90004436
Si	0.96530830	-0.60455252	-1.76396387
O	1.69271118	0.79268908	-1.28170991
O	0.28105566	-1.32827735	-0.45202504
O	-2.43487205	-1.36874527	-0.49577347
Si	-3.34088636	-0.13325406	-1.14641754
O	-2.81855232	0.16769049	-2.68686776
O	2.07645000	-1.60226230	-2.41525153
O	-2.97946977	1.20074864	-0.24123310
O	0.61310432	3.20148885	-0.77614225
O	-0.64070965	4.87917311	-2.45233978
O	-1.51666753	0.91849992	-4.89955382
Si	-1.31076367	6.42878875	-2.43297737
Si	-1.35538759	2.19933414	-5.98942560
Si	1.23722413	1.25107609	4.59120063
Si	-2.12191951	-3.93402987	2.02898058
H	-1.30208636	-4.81502162	2.90574460
H	-3.00178967	-3.05169583	2.85729467
H	-2.96599918	-4.74701941	1.10597305
H	1.88136243	2.56857287	4.31320835
H	0.81111063	1.16786428	6.01603116
H	2.18326660	0.14483904	4.26344817
H	-0.00307896	2.81343378	-5.84720715
H	-1.52486935	1.61832181	-7.35024840
H	-2.41057561	3.22014037	-5.72173785
H	-1.06177640	7.06746872	-1.10797783
H	-0.63053141	7.19191185	-3.51645024
H	-2.77650728	6.34364233	-2.69599379
Si	3.90202433	3.08045122	1.52502056
H	3.13976909	4.14600075	2.24040355
H	4.11193464	1.91506190	2.43349984
H	5.20598386	3.60536844	1.03471664
Si	2.37603412	-2.26605586	-3.93915770
H	1.19751906	-3.06659923	-4.37980410
H	2.64751053	-1.17192860	-4.91682767
H	3.57387841	-3.13811130	-3.78787539
H	-5.83993192	1.36185355	-2.93162926
O	-4.91106579	-0.47031950	-1.07466724
H	-4.88870093	2.82147065	0.83799771
O	-4.08263972	3.20950432	1.20711575
H	-6.36818038	1.88812523	-2.91013457
H	-7.69688772	-0.38618909	-0.58887023
H	-6.13599315	1.72899540	0.25059543
Al	-6.27723648	0.17280379	-0.13821380
N	-5.97635777	-0.72296421	1.68670718
C	-5.88881642	-2.18537298	1.48733011
H	-5.04883803	-2.40844739	0.82869522
H	-5.74985136	-2.69123773	2.44864833
H	-6.80710577	-2.54531690	1.02068477
C	-7.13615413	-0.39717478	2.54200684
H	-7.19824790	0.68437970	2.67622067
H	-8.05205456	-0.75136063	2.06705980
H	-7.03038897	-0.87296375	3.52255100
C	-4.73768246	-0.23260682	2.32814313
H	-3.87457149	-0.48739044	1.71422685
H	-4.78767523	0.85057447	2.44384300
H	-4.61346549	-0.69280808	3.31407692

AC_$AlH_2 \cdot NMe_3$

E: -1749.83286459 ; H: -1749.368999 ; G: -1749.523009

O	-0.15763069	0.62707906	4.17126831
Si	-0.43569732	0.77433951	2.57040603
O	0.41364827	2.05335679	1.97004035
Si	1.16461418	2.58925166	0.60639764
O	2.41159041	3.55486119	1.02176865
O	0.04715244	-0.60355370	1.80172100
Si	-0.26022355	-1.59546412	0.51886439
O	0.15936051	-3.12489808	0.90754297
O	-2.04721921	1.02592203	2.34413380
Si	-3.10098085	1.67421919	1.24858230
O	-2.41134242	3.02274264	0.59017628
Si	-1.51052640	3.50519208	-0.70271977
O	-1.80855796	2.52925534	-1.99962341
Si	-1.30753117	1.14127839	-2.74185192
O	0.31208889	0.95125489	-2.49738721
Si	1.35155888	0.23302736	-1.44176677
O	1.74906471	1.30624069	-0.25495181
O	0.64649633	-1.09998252	-0.76619784
O	-1.86404697	-1.55100114	0.15007418
Si	-2.93821844	-0.71564995	-0.79778117
O	-2.11270506	-0.14681217	-2.11646735
O	2.70509551	-0.22060999	-2.23024296
O	-4.52843922	2.04313904	1.98193676
O	-3.46752810	0.59479176	0.07514684
O	0.08897863	3.43163784	-0.31287164
O	-4.17588515	-1.64312287	-1.22642741
O	-1.91322292	5.03953053	-1.08245955
O	-1.59202234	1.25450017	-4.34334592
H	-4.48141403	2.66533941	2.70894722
Si	-2.17554794	5.91333777	-2.50173704
Si	-2.80775567	0.77451324	-5.41370261
Si	0.97194322	-0.18324392	5.13024464
Si	-0.68799419	-4.56800130	1.13544046
H	0.29615942	-5.55413329	1.66285321
H	-1.78757080	-4.35526786	2.12222373
H	-1.24936142	-5.03530546	-0.16498787
H	0.97954587	0.50144595	6.45293561
H	0.55665714	-1.60794589	5.28226920
H	2.31944428	-0.10820829	4.49352482
H	-2.29574947	1.06788080	-6.78235680
H	-3.07335937	-0.68426719	-5.25332650
H	-4.04777701	1.55758194	-5.14276801
H	-2.20161760	7.35141753	-2.11492141
H	-1.07181915	5.65157536	-3.47109885
H	-3.48341617	5.51175350	-3.09738976
Si	4.04917364	3.63952581	0.61651057
H	4.58912519	4.84879442	1.29824320
H	4.74861080	2.41343679	1.09962077
H	4.19596020	3.76244902	-0.86281774
Si	3.52588514	-1.67315859	-2.48849656
H	2.60323766	-2.67336286	-3.09982350
H	4.64863385	-1.36161119	-3.41639946
H	4.04978441	-2.18935361	-1.19023092
H	-5.99962896	-2.99286173	-2.90701818
H	-5.54031681	-0.28646994	-3.31334919
Al	-5.55731985	-1.56358921	-2.34613539
N	-7.06759902	-1.11236338	-1.03496347
C	-6.81745700	0.20392274	-0.40980753
H	-5.88076648	0.17601333	0.14497242
H	-6.74296318	0.96694707	-1.18591946
H	-7.63546950	0.46012027	0.27220092
C	-8.33527723	-1.07615594	-1.79010737
H	-8.50508322	-2.04326316	-2.26628323
H	-9.17188633	-0.85233771	-1.11929536
H	-8.27834610	-0.30443099	-2.55982157
C	-7.13146342	-2.15561024	0.00904089

H	-7.32015016	-3.12442071	-0.45590855
H	-6.17789368	-2.19528770	0.53584631
H	-7.93357711	-1.93201854	0.72086816

B^{0}_AlH_2·NMe_3 _TS_HH adduct

E: -1749.83281142 ; H: -1749.368777 ; G: -1749.518749

O	0.23162519	0.91002728	3.51545706
Si	-0.22836804	0.97110835	1.95129428
O	0.87508498	1.81865084	1.07639665
Si	1.63744788	2.58007344	-0.16306086
O	2.78596930	3.58768065	0.40179704
O	-0.32927239	-0.57664947	1.37102276
Si	-0.06036934	-1.56441845	0.08330678
O	0.32525482	-3.04522904	0.65048616
O	-1.69088223	1.72948662	1.85085705
Si	-2.61968372	2.02924058	0.51154919
O	-2.01425946	3.36304720	-0.27956161
Si	-0.99403300	3.59363932	-1.55289328
O	-1.31347367	2.52117965	-2.77338365
Si	-0.93571095	1.05608530	-3.42453657
O	0.56173223	0.58670884	-2.92983601
Si	1.76119027	0.10915643	-1.91349426
O	2.34462607	1.43109050	-1.12149279
O	1.19397507	-0.98782560	-0.82086096
O	-1.40366533	-1.68999835	-0.87666693
Si	-2.48201979	-0.57558488	-1.44521897
O	-2.03666570	-0.09470771	-2.97154365
O	2.97453756	-0.57463229	-2.76421053
O	-4.17389245	2.22959411	0.86873836
O	-2.33565913	0.76652788	-0.51576197
O	0.56794656	3.45210649	-1.05860695
O	-1.25280062	5.09677983	-2.14599261
O	-0.96912967	1.20644421	-5.05018289
Si	-1.70735887	5.68953726	-3.65827913
Si	-0.92909093	0.15301497	-6.36776635
Si	0.59475408	-0.31382976	4.61953898
Si	0.38393060	-4.62087680	0.05257724
H	1.11387018	-5.43421320	1.06442469
H	-1.00167784	-5.13842861	-0.13652518
H	1.11696774	-4.63309152	-1.24929664
H	0.99846292	0.36544625	5.88224654
H	-0.61041193	-1.16333237	4.84672957
H	1.71542488	-1.14836835	4.09564213
H	-0.25108702	0.87161903	-7.48295052
H	-0.17110978	-1.08142103	-6.00565766
H	-2.32691028	-0.19870197	-6.75167882
H	-1.69237528	7.17528062	-3.55420627
H	-0.75673985	5.22204977	-4.70710548
H	-3.08827205	5.21505763	-3.97945570
Si	4.35463000	3.45123483	1.00914794
H	4.52856892	4.53429646	2.01704079
H	4.53515091	2.11245316	1.64511666
H	5.32386106	3.61990644	-0.11103886
Si	3.49522377	-2.15900203	-3.02636340
H	2.33938816	-3.00332191	-3.45261124
H	4.52052386	-2.09628824	-4.10420668
H	4.08473278	-2.70791501	-1.77055800
N	-6.10543591	3.63764398	-0.88490324
C	-6.15860476	4.75072830	0.08766174
H	-5.20408910	4.81686968	0.61073124
H	-6.35602953	5.69587543	-0.42902156
H	-6.95128980	4.56394450	0.81357595
C	-5.03810486	3.89882461	-1.87552654
H	-4.09510288	4.05820562	-1.35395109
H	-4.93995046	3.04463636	-2.54786542
H	-5.28136056	4.79170092	-2.46104741

C	-7.40627636	3.50305249	-1.57240188
H	-7.35368821	2.68993263	-2.29856352
H	-8.18556349	3.28044207	-0.84155093
H	-7.65793673	4.43256709	-2.09367268
O	-3.97730833	-1.24377095	-1.43386719
H	-4.69660354	-0.60041632	-1.37029511
H	-5.65147742	0.84285376	-1.09468211
H	-6.96754426	1.79623730	1.13807022
Al	-5.74799225	1.89749217	0.12223508

B^{0}_$AlH_2{\cdot}NMe_3$ _TS_HH TS

E: -1749.80136550 ; H: -1749.341769 ; G: -1749.486634

O	0.05957988	1.30614372	3.43653695
Si	-0.24178575	1.32478655	1.83170747
O	1.05930691	1.93451775	1.02914986
Si	1.86049968	2.52489179	-0.27924799
O	3.12008707	3.43732723	0.21168559
O	-0.52559843	-0.23979596	1.35483293
Si	-0.40443233	-1.30002240	0.09833883
O	-0.19322721	-2.78962201	0.73427216
O	-1.54561002	2.31823959	1.56934928
Si	-2.28900269	2.52446394	0.10126301
O	-1.71756239	3.85872523	-0.70541826
Si	-0.56309576	3.83231643	-1.89660337
O	-0.93834989	2.76713617	-3.11607210
Si	-0.71757247	1.22059103	-3.64609608
O	0.71412722	0.61018078	-3.10834361
Si	1.70704823	-0.00114257	-1.94945704
O	2.43477165	1.24716713	-1.15869332
O	0.87988907	-0.93090167	-0.86869818
O	-1.77273568	-1.32993823	-0.85576757
Si	-2.42685153	0.00611221	-1.58019436
O	-1.94180472	0.19828684	-3.15479588
O	2.85803997	-0.91961437	-2.65416403
O	-3.89715706	2.49463597	0.18055203
O	-1.67177936	1.26286502	-0.80002601
O	0.89118542	3.44583802	-1.23178297
O	-0.49428406	5.32496806	-2.55813925
O	-0.72196579	1.26333391	-5.27949396
Si	-0.38728363	5.91298194	-4.13647750
Si	-0.72275250	0.12398937	-6.52307489
Si	0.43440658	0.11352327	4.56971507
Si	-0.16603916	-4.37317253	0.15524478
H	0.54911438	-5.19202401	1.17328205
H	-1.56293206	-4.86361565	-0.02379112
H	0.56298600	-4.41526239	-1.14848298
H	0.83367912	0.82544384	5.81593874
H	-0.76471661	-0.73809306	4.81943074
H	1.56118960	-0.72716927	4.06792920
H	-0.03179482	0.74574101	-7.68692212
H	-0.00136661	-1.10705408	-6.08255449
H	-2.13275418	-0.21138858	-6.87840291
H	-0.08345054	7.36729019	-4.02785675
H	0.69979054	5.20476327	-4.87335091
H	-1.69135518	5.70892395	-4.83380602
Si	4.69323941	3.18119243	0.75893596
H	4.99142095	4.24797049	1.75575882
H	4.79747415	1.83379124	1.39429125
H	5.63186167	3.27412899	-0.39626005
Si	3.28363969	-2.55107848	-2.65016096
H	2.22641965	-3.34493053	-3.34369152
H	4.57506966	-2.65497667	-3.38463068
H	3.43781142	-3.03397594	-1.24631651
N	-6.55706995	3.11237946	-0.45181235
C	-6.71577387	3.57609016	0.94180287
H	-5.75134318	3.91110508	1.32260763

H	-7.43515154	4.40094588	0.98817227
H	-7.07651905	2.75247206	1.56037901
C	-6.03574666	4.21240795	-1.28629633
H	-5.06950440	4.53279946	-0.89792592
H	-5.90863433	3.86204918	-2.31205597
H	-6.73284749	5.05748527	-1.28074927
C	-7.85915964	2.65769208	-0.97322837
H	-7.74180289	2.31395071	-2.00229446
H	-8.22684154	1.83113456	-0.36295579
H	-8.58888704	3.47431030	-0.94976207
O	-4.05269031	0.08536275	-1.42408417
H	-4.78343936	0.77698777	-2.11421119
H	-5.50018451	1.49092692	-2.20538659
H	-6.09658269	0.52586186	0.47199049
Al	-5.23759581	1.50005930	-0.43034132

B^{0}_$AlH_2{\cdot}NMe_3$ _TS_HH product / H_2 adduct

E: -1749.86597608 ; H: -1749.404617 ; G: -1749.553352

O	0.57242062	1.16725845	3.65533788
Si	0.04620404	1.30184792	2.11490789
O	1.25163194	1.89587759	1.16686705
Si	1.87444248	2.56013368	-0.20275588
O	3.21788916	3.41066942	0.15569072
O	-0.39483021	-0.21532256	1.60328527
Si	-0.48307665	-1.19904526	0.28163643
O	-0.24935084	-2.73102705	0.79920776
O	-1.22271433	2.37290454	2.09531836
Si	-2.17556516	2.67845137	0.77464870
O	-1.69057847	4.03875395	-0.05010954
Si	-0.70084160	4.04063409	-1.38242295
O	-1.28705816	3.06484461	-2.59277249
Si	-1.21246213	1.54041093	-3.22591557
O	0.25046937	0.84738126	-2.93424569
Si	1.38001736	0.14825316	-1.96352001
O	2.26509522	1.33349583	-1.24054665
O	0.68495257	-0.80761852	-0.81552295
O	-1.96264842	-1.12935604	-0.48186663
Si	-2.67839663	0.27078371	-1.00568648
O	-2.40623096	0.54626456	-2.62353825
O	2.37681501	-0.77188580	-2.87315064
O	-3.76098025	2.67971588	1.08599962
O	-1.75410564	1.45314388	-0.27949925
O	0.80976792	3.57067130	-0.93923842
O	-0.66467685	5.56541482	-1.97044578
O	-1.44863900	1.68718595	-4.83687395
Si	-0.84134403	6.24578152	-3.50368311
Si	-1.70887636	0.63611449	-6.12921607
Si	0.84745344	-0.12154180	4.70925443
Si	-0.43707401	-4.28502021	0.17368002
H	0.18551246	-5.21947391	1.15248133
H	-1.88735100	-4.59090672	0.00777785
H	0.25874622	-4.37717632	-1.14543133
H	1.36922544	0.47183680	5.97266972
H	-0.42900834	-0.85000352	4.96589495
H	1.85565105	-1.05063256	4.11961051
H	-1.02538758	1.21953441	-7.31737442
H	-1.14821856	-0.71064188	-5.81094741
H	-3.17616703	0.53206593	-6.37944490
H	-0.52775735	7.69516726	-3.36411802
H	0.09510959	5.59600600	-4.46606907
H	-2.25000557	6.06700331	-3.96831201
Si	4.77080301	3.11300144	0.73982373
H	5.06816833	4.14735724	1.77066982
H	4.83408507	1.74800586	1.34148489
H	5.73374010	3.21846294	-0.39348526

Si	2.64249766	-2.42755382	-3.05865452
H	1.37536208	-3.09504937	-3.48284744
H	3.68381977	-2.57384710	-4.11294913
H	3.11503910	-3.01243533	-1.77000231
N	-5.79599741	2.89475303	-1.04002017
C	-6.31498652	4.09966213	-0.35531874
H	-5.49427812	4.60192011	0.15770097
H	-6.76420771	4.78358249	-1.08250152
H	-7.06953685	3.80653661	0.37680206
C	-4.75280057	3.28393736	-2.01489504
H	-3.94223670	3.79502521	-1.49536746
H	-4.36728642	2.39254713	-2.50922693
H	-5.17366858	3.95949813	-2.76647093
C	-6.89492134	2.19313521	-1.73863318
H	-6.49894940	1.30730078	-2.23672424
H	-7.65276605	1.88858205	-1.01510792
H	-7.35060495	2.85407870	-2.48273825
O	-4.24349444	0.40168278	-0.61920470
H	-5.28874509	-0.72728045	-2.65087618
H	-5.59634390	-1.03695989	-3.25618132
H	-6.25230550	1.23575308	1.27649567
Al	-5.03284431	1.65785719	0.36995708

B^{0}_AlH·NMe$_3$

E: -1748.68855793 ; H: -1748.243079 ; G: -1748.388587

O	0.22606762	0.87456383	3.79859836
Si	-0.16992054	1.08254368	2.22916167
O	1.10142691	1.74611945	1.42144320
Si	1.81281449	2.42648143	0.11034566
O	3.13823315	3.24209611	0.59950334
O	-0.54072712	-0.40849301	1.60067252
Si	-0.55870045	-1.34061405	0.24017793
O	-0.34665462	-2.88951439	0.71240752
O	-1.45252894	2.13503891	2.15698398
Si	-2.30214968	2.49976039	0.78341589
O	-1.76180525	3.89820048	0.06134102
Si	-0.68191642	3.95273389	-1.19872191
O	-1.18730218	3.03861368	-2.49136571
Si	-1.03959300	1.54711260	-3.18879645
O	0.41862705	0.87305925	-2.83582378
Si	1.45351596	0.10680352	-1.81187419
O	2.27560912	1.23874592	-0.94303240
O	0.65977811	-0.90587456	-0.78384915
O	-1.99438154	-1.24474527	-0.60087480
Si	-2.66202755	0.17593547	-1.13571393
O	-2.24798253	0.50367919	-2.71437395
O	2.51948045	-0.76894711	-2.68594526
O	-3.90730961	2.48781893	0.97257304
O	-1.79765407	1.32836534	-0.29435900
O	0.79309324	3.45119954	-0.67867175
O	-4.25223441	0.30093750	-0.87846622
O	-0.59636340	5.50319939	-1.71062113
O	-1.17668107	1.76692859	-4.80365602
Si	-0.76315290	6.26905645	-3.20381888
Si	-1.43845343	0.77010998	-6.13851528
Si	0.48796726	-0.45386502	4.80521626
Si	-0.56287819	-4.42478909	0.05059992
H	0.04618373	-5.39145520	1.00635598
H	-2.01885265	-4.70169833	-0.11671212
H	0.12730800	-4.49893704	-1.27246308
H	0.96141199	0.09152131	6.10852037
H	-0.78728486	-1.20566004	4.99013480
H	1.52509977	-1.34638989	4.20981747
H	-0.73684601	1.39257228	-7.29578074
H	-0.89708053	-0.59492073	-5.86902707
H	-2.90449330	0.69274976	-6.40649508

H	-0.45672313	7.70881937	-2.97801976
H	0.18480844	5.67890096	-4.19325571
H	-2.16669432	6.11151988	-3.69149569
Si	4.56547096	3.78987276	-0.11366970
H	4.99032049	5.00434656	0.63742750
H	5.60469095	2.72553356	-0.01131220
H	4.31723052	4.12559244	-1.54752798
Si	2.86323287	-2.41287392	-2.84827243
H	1.63913046	-3.13957682	-3.30097278
H	3.93859545	-2.52065397	-3.87268031
H	3.32505469	-2.96616918	-1.54212862
H	-6.41002916	1.05143712	0.88130992
Al	-5.11780495	1.51170368	0.10298284
N	-5.75905039	2.81693643	-1.30527187
C	-6.41830933	3.94625667	-0.61293636
H	-5.69601218	4.44008589	0.03807901
H	-6.80170200	4.66539358	-1.34377210
H	-7.24658694	3.57149083	-0.00908141
C	-4.62381679	3.31927241	-2.11082550
H	-3.90957963	3.82135352	-1.45875861
H	-4.13822891	2.48390318	-2.61450791
H	-4.98211978	4.03051485	-2.86167556
C	-6.72662381	2.12454550	-2.18409454
H	-6.23015670	1.29112087	-2.68257329
H	-7.55508491	1.74155762	-1.58581896
H	-7.11701384	2.81833846	-2.93566978

Bipodal site B*1*

B*1*

E: -1659.33388314 ; H: -1658.943376 ; G: -1659.093481

O	-0.82249178	0.44950109	3.69655307
Si	-0.79657296	0.60371109	2.07265043
O	0.49394267	1.54632011	1.64475101
Si	1.43310062	1.95639494	0.35648837
O	2.84738572	2.55557625	0.89936788
O	-0.62880152	-0.89929227	1.41866595
Si	-0.99147326	-1.75037739	0.05615648
O	-1.06695672	-3.33834951	0.42269359
O	-2.18174116	1.26492293	1.49426942
Si	-2.93914748	2.68899773	1.12332933
O	-1.87558215	3.64566291	0.25830930
Si	-0.89956592	3.34657292	-1.02955989
O	-1.47061189	1.94345204	-1.71843370
Si	-1.12787834	1.02406721	-3.04760640
O	0.41253986	0.43104394	-2.91910146
Si	1.20814179	-0.41015625	-1.73684799
O	1.73582470	0.62092295	-0.56951148
O	0.17783025	-1.52564432	-1.08565871
O	-2.43218650	-1.23387120	-0.54959710
Si	-3.24340775	-0.87541519	-1.92993812
O	-2.21745116	-0.21161750	-3.04978163
O	2.48190367	-1.18484130	-2.39570587
O	-3.29709622	3.53358182	2.48186433
O	-4.31128049	2.36793916	0.29462275
O	0.65872774	3.10083847	-0.54917324
O	-3.94793208	-2.18358281	-2.61516782
O	-0.89379666	4.58243639	-2.09318163
O	-1.24124072	1.89884539	-4.42005948
Si	-2.85836979	5.04444123	3.08610751
Si	-3.40582389	-3.51562076	-3.50855352
Si	-1.96545663	5.27334133	-3.20088136
Si	-0.21324964	2.29554940	-5.70669165
Si	-0.63087526	1.45869686	5.03446004
Si	-0.83904894	-4.27081799	1.81310258
H	-1.10856671	-5.68182774	1.41922487
H	0.56818775	-4.12195111	2.28637435

H	-1.78775125	-3.83142800	2.87604633
H	-1.70333643	1.11916611	6.01100411
H	0.71417381	1.21296747	5.62826827
H	-0.75118761	2.88502742	4.60741288
H	0.93723876	3.09211484	-5.19168454
H	0.26883017	1.04364970	-6.35759724
H	-1.02861566	3.10324310	-6.65503219
H	-2.12659930	6.71084972	-2.84453171
H	-1.36594348	5.14181053	-4.56016239
H	-3.27784362	4.56627428	-3.14156334
H	-3.47015680	5.15173229	4.44122264
H	-1.37202491	5.14314605	3.18540519
H	-3.38032844	6.12145874	2.19444183
H	-4.40479769	-4.60188932	-3.31149553
H	-3.32074037	-3.13524956	-4.94770048
H	-2.06392751	-3.93132033	-3.00438926
H	-4.29954634	1.59736721	-0.29515539
O	-4.42439171	0.20338472	-1.47409999
H	-5.20782356	0.22851851	-2.02671248
Si	2.98680443	-2.79667811	-2.46302872
H	4.28926776	-2.79900118	-3.18439331
H	3.15204527	-3.32738944	-1.07819188
H	1.97535013	-3.60584796	-3.20281069
Si	4.46187308	2.51198036	0.40854429
H	5.16734283	3.57903887	1.17097079
H	5.04012622	1.17406044	0.72605916
H	4.54830561	2.76964328	-1.05869430

B^{1}_AlH_3_NMe_3_TS_HH (N/O *trans*) adduct

E: -1837.66392807 ; H: -1837.118015 ; G: -1837.282411

O	-1.17629665	1.09235253	4.29903347
Si	-1.40707633	1.35406091	2.70532727
O	-0.03781833	2.00573727	2.05135243
Si	0.77238088	2.21363637	0.62814527
O	2.35542505	2.43570207	0.94473049
O	-1.75072627	-0.08597040	2.00075850
Si	-2.47080587	-0.82987223	0.71814431
O	-2.82341049	-2.36706938	1.13688759
O	-2.66046463	2.40607089	2.44415849
Si	-2.76035363	4.04969172	2.38851147
O	-1.87742138	4.68172849	1.15860825
Si	-1.33574519	4.19470787	-0.32327137
O	-2.34133074	3.00334161	-0.87623682
Si	-2.47963415	2.09027396	-2.24867507
O	-1.13655668	1.12589858	-2.36665901
Si	-0.34526944	0.05592184	-1.39023996
O	0.59974071	0.86645210	-0.31301833
O	-1.44079767	-0.87754325	-0.57566821
O	-3.80990758	0.01402494	0.27895993
Si	-4.69048664	0.20050134	-1.11796313
O	-3.84293869	1.19470190	-2.14650983
O	0.58812534	-0.91875925	-2.30658707
O	-2.23809322	4.66165679	3.81765610
O	0.17378244	3.53939339	-0.14884046
O	-4.90212787	-1.24404370	-1.86278252
O	-1.19180590	5.45228792	-1.34245364
O	-2.57333632	3.02844876	-3.58304856
Si	-1.19835821	5.91844549	4.27709335
Si	-4.05424360	-2.20886314	-2.95224869
Si	-2.05017391	6.72725394	-2.03425502
Si	-1.56211104	3.65323422	-4.77877883
Si	-0.89018672	1.98120152	5.70389095
Si	-2.77800657	-3.29285334	2.54725755
H	-3.41099118	-4.60003219	2.21649869
H	-1.35986356	-3.49195067	2.96635734
H	-3.53843999	-2.60248116	3.62911263

H	-2.18218605	2.50417253	6.23199148
H	-0.26801911	1.04524423	6.68148655
H	0.03963594	3.11104140	5.40476947
H	-0.49941603	4.48553597	-4.14313587
H	-0.95173941	2.53723468	-5.55703420
H	-2.42267421	4.49585004	-5.65653817
H	-2.66803710	7.57883339	-0.98080757
H	-1.04686455	7.50849328	-2.81337387
H	-3.08987575	6.18503080	-2.95841730
H	-1.21038091	5.94194224	5.76644729
H	0.17308737	5.63556316	3.76581520
H	-1.70696682	7.20742982	3.72579198
H	-3.56308779	-3.41932202	-2.23355902
H	-4.99140154	-2.59927398	-4.04443273
H	-2.89825127	-1.44603554	-3.51222079
O	-6.16253601	0.83798672	-0.78210524
H	-6.09319222	1.71067820	-0.35151861
Si	0.67244350	-2.58568935	-2.56914774
H	1.72263751	-2.79462147	-3.60422397
H	1.04447752	-3.27515398	-1.29920183
H	-0.64785748	-3.08453372	-3.05251279
Si	3.81605754	1.81122268	0.37385620
H	4.89022330	2.69203986	0.91059032
H	3.98792593	0.41545991	0.87157062
H	3.82321264	1.82533911	-1.11810200
H	-4.98048105	4.33124034	2.81269570
O	-4.34834931	4.49345952	2.10758080
H	-4.12076843	5.33875578	-0.50074785
H	-5.62977459	3.09112786	0.17539610
H	-6.53786445	5.57452975	0.91381785
Al	-5.46747049	4.69464334	0.08712428
N	-6.51022925	4.82950965	-1.77118444
C	-5.76610243	4.06721620	-2.78719458
H	-4.75110171	4.45780946	-2.86775821
H	-5.71563965	3.01882527	-2.49291101
H	-6.25703928	4.13982925	-3.76563919
C	-7.86623812	4.27967008	-1.62496736
H	-8.42610403	4.37452261	-2.56360529
H	-7.80431395	3.22393265	-1.35743383
H	-8.39437769	4.81530344	-0.83443720
C	-6.57965302	6.24663037	-2.15684394
H	-7.10956465	6.80913841	-1.38622433
H	-5.56842437	6.64607495	-2.25090264
H	-7.10182350	6.36535245	-3.11445082

B*1*_AlH$_3$_NMe$_3$_TS_HH (N/O *trans*) TS

E: -1837.63786184 ; H: -1837.095960 ; G: -1837.261776

O	-1.05970088	1.08861890	4.29502027
Si	-1.30571651	1.31812745	2.69828596
O	0.06931973	1.93445175	2.02095907
Si	0.82077596	2.13881001	0.56959253
O	2.41505338	2.36883251	0.81971462
O	-1.64986156	-0.14237502	2.01959068
Si	-2.43535131	-0.85155796	0.76069057
O	-2.82759228	-2.38068338	1.17038284
O	-2.56579944	2.33625515	2.41055587
Si	-2.86296799	3.95838255	2.27034834
O	-1.78866056	4.63128420	1.19137884
Si	-1.28074287	4.19626123	-0.31105460
O	-2.38716121	3.10830420	-0.90544762
Si	-2.52735506	2.11767848	-2.22195142
O	-1.19603276	1.14209788	-2.31901178
Si	-0.38579167	0.02345611	-1.41499955
O	0.62069054	0.78270536	-0.35845694
O	-1.46590847	-0.91335975	-0.58132399
O	-3.76571890	0.03793711	0.36094687

Si	-4.66726650	0.18386873	-1.02468937
O	-3.89916662	1.23973557	-2.05002021
O	0.47823175	-0.93732475	-2.40932944
O	-2.58877532	4.68651893	3.71563459
O	0.18718663	3.44420346	-0.21129724
O	-4.83894559	-1.25485874	-1.78308951
O	-1.07400622	5.47848635	-1.29161435
O	-2.64734957	2.98711790	-3.60068361
Si	-1.68335842	6.01186671	4.23594429
Si	-3.93872813	-2.21068073	-2.84262706
Si	-1.85386576	6.75058684	-2.06840507
Si	-1.61940541	3.61676328	-4.78124688
Si	-0.99902407	2.03350036	5.69316813
Si	-2.79694686	-3.31806136	2.57488146
H	-3.47711257	-4.60027300	2.24044463
H	-1.38140117	-3.56644449	2.97480214
H	-3.52357839	-2.61077750	3.66888626
H	-2.38588669	2.33729261	6.14562384
H	-0.27434844	1.23067575	6.71754276
H	-0.25920324	3.29983275	5.41211562
H	-0.55521115	4.43137740	-4.12462092
H	-1.01156764	2.50362745	-5.56503908
H	-2.46530220	4.47606199	-5.65683797
H	-2.40016642	7.71531557	-1.07498534
H	-0.81934320	7.40683538	-2.91843637
H	-2.94522367	6.21328317	-2.93636816
H	-1.91604962	6.13131829	5.70323046
H	-0.23594954	5.77584910	3.96017670
H	-2.14378765	7.24630706	3.53414861
H	-3.35236022	-3.34847668	-2.07934541
H	-4.86798235	-2.70978857	-3.89533411
H	-2.85112661	-1.39041986	-3.45542334
O	-6.17006187	0.74483204	-0.65563218
H	-6.16114298	1.55015780	-0.12636723
Si	0.63471751	-2.60365854	-2.64025136
H	1.68408778	-2.78663774	-3.68063373
H	1.04414068	-3.25269595	-1.36085086
H	-0.66693930	-3.16532089	-3.10514922
Si	3.85179734	1.74133822	0.19535042
H	4.94914877	2.61064099	0.70332264
H	4.03214067	0.33969573	0.67320782
H	3.81061168	1.76907693	-1.29609576
H	-5.00328317	3.35753629	1.02502607
O	-4.41347886	4.13378409	1.76423973
H	-4.05240443	5.67480488	-0.48510770
H	-5.59699984	3.20786132	0.22336415
H	-6.48209095	5.84151053	1.00126067
Al	-5.33979163	5.04889760	0.22102192
N	-6.41664638	4.91016300	-1.60276369
C	-5.65504846	4.13358398	-2.59672764
H	-4.66583918	4.57343211	-2.72457412
H	-5.54535831	3.10573111	-2.25226266
H	-6.17332329	4.12834524	-3.56267770
C	-7.74381809	4.30455105	-1.40244478
H	-8.32494985	4.33628563	-2.33135470
H	-7.62859025	3.26309254	-1.10031641
H	-8.27986842	4.84576311	-0.62135797
C	-6.57014283	6.29966644	-2.06967489
H	-7.12525152	6.87660176	-1.32796373
H	-5.58478820	6.74929731	-2.20518533
H	-7.10971588	6.32744668	-3.02328235

B^{1}_AlH_3_NMe_3_TS_HH (N/O *trans*) product / H_2 adduct

E: -1837.70130230 ; H: -1837.157830 ; G: -1837.327302 ;

O	-2.17776584	1.86635875	3.88656033
Si	-2.09127507	1.89949128	2.25803334

O	-0.50583365	2.04815109	1.81049425
Si	0.49133257	2.31362910	0.52944893
O	2.03198422	2.42655277	1.05219152
O	-2.68915858	0.46824189	1.70106766
Si	-3.08269563	-0.35254450	0.33517795
O	-3.68406893	-1.81073343	0.75994196
O	-2.98264229	3.10955524	1.58908717
Si	-2.88064093	4.77601867	1.60187046
O	-2.14697101	5.20665016	0.15596080
Si	-1.25081174	4.37847806	-0.94305329
O	-2.15602882	3.14236789	-1.56691317
Si	-2.25935618	2.18250098	-2.90817735
O	-1.15102178	0.96375224	-2.74272279
Si	-0.52708971	0.08650657	-1.49167796
O	0.39383370	1.04482762	-0.52567672
O	-1.75486886	-0.59679675	-0.62008508
O	-4.19592288	0.50113623	-0.53415101
Si	-4.69205654	0.48258867	-2.11768979
O	-3.78057263	1.55813991	-2.97323963
O	0.40148393	-1.10375394	-2.10942910
O	-1.85591883	5.17245223	2.83517269
O	0.08442108	3.71908957	-0.22909981
O	-4.58694528	-1.03694605	-2.72056277
O	-0.78002534	5.39073236	-2.13901654
O	-1.99299387	3.00648910	-4.28565802
Si	-0.46305447	6.10920202	2.99303437
Si	-3.51798751	-2.17119179	-3.36762419
Si	-0.92499379	7.05320523	-2.42819183
Si	-0.71609143	3.75153584	-5.10486288
Si	-1.60045425	2.77141281	5.19009444
Si	-3.73918981	-2.73015722	2.17520622
H	-4.35395017	-4.03549257	1.80372804
H	-2.35489092	-2.93579120	2.69397396
H	-4.57178089	-2.03144065	3.19572145
H	-2.60103190	3.81264694	5.55431452
H	-1.41433144	1.81382068	6.31756415
H	-0.29433516	3.39969297	4.83296067
H	0.55926043	3.53333121	-4.36413657
H	-0.64325755	3.13459508	-6.46013950
H	-1.02149312	5.20556410	-5.21735007
H	-0.48144185	7.81062597	-1.22225984
H	-0.04165577	7.35010998	-3.59009000
H	-2.34421295	7.37466082	-2.75335027
H	-0.21445357	6.26907223	4.45356416
H	0.68348091	5.40705417	2.34542915
H	-0.67252037	7.44144754	2.35176311
H	-3.27291725	-3.22502776	-2.34350932
H	-4.16798901	-2.75664580	-4.57440302
H	-2.24079900	-1.49665414	-3.73774050
O	-6.25170668	1.01631931	-2.22056994
H	-6.92550427	0.34447974	-2.10702051
Si	0.65801967	-2.73699671	-1.76905783
H	1.87169982	-3.14539985	-2.52895204
H	0.86974418	-2.91968161	-0.30287262
H	-0.52786707	-3.52676699	-2.21373245
Si	3.42233742	1.48162456	0.89853628
H	4.48776909	2.16742055	1.68054406
H	3.16501399	0.11846048	1.45050162
H	3.80773365	1.38291558	-0.53894311
H	-6.76555729	0.02892373	1.53070713
O	-4.33493226	5.42975621	1.73162225
H	-5.47608037	7.19661963	-0.17094488
H	-6.24551803	0.20622936	1.02670951
H	-7.03040247	6.18655668	1.88617881
Al	-5.77748335	6.04655716	0.90166345
N	-6.31621430	4.47173334	-0.29293359
C	-5.28129170	4.23270389	-1.32276338

H	-5.05026255	5.16816233	-1.83521349
H	-4.37930018	3.84804372	-0.85059204
H	-5.63836834	3.49676527	-2.04801884
C	-6.49674610	3.24360301	0.51349919
H	-6.79405336	2.41524266	-0.13526177
H	-5.55635666	2.99240705	1.00457819
H	-7.26348575	3.41468364	1.27108584
C	-7.58743139	4.83448341	-0.95044850
H	-8.35207936	5.01897774	-0.19406440
H	-7.44505239	5.74116775	-1.54158530
H	-7.91678025	4.02501115	-1.61013295

B^{1}_AlH_3_NMe_3_TS_HH (N/O *cis*) adduct

E: -1837.66724765 ; H: -1837.120748 ; G: -1837.285424

O	-0.92885791	1.25855541	3.65049392
Si	-1.03435014	0.99842864	2.04307469
O	0.42282014	1.32235977	1.33274082
Si	1.11013157	1.87691392	-0.06518520
O	2.56114184	2.53077671	0.29282849
O	-1.43246874	-0.58251322	1.81665284
Si	-1.50391584	-1.62194032	0.54392815
O	-1.67596763	-3.12947555	1.14611652
O	-2.20938926	1.91430353	1.34060832
Si	-2.59338572	3.50894427	1.08858135
O	-2.39819102	3.78373030	-0.54205742
Si	-1.28386928	3.10674130	-1.55672060
O	-1.72643694	1.57090659	-1.93740430
Si	-1.70424506	0.41598638	-3.11669906
O	-0.39028601	-0.56059567	-2.84226615
Si	0.66802306	-0.80912108	-1.59805945
O	1.30526783	0.63614347	-1.12926683
O	-0.10846224	-1.53233880	-0.33509476
O	-2.78954651	-1.18670347	-0.39670082
Si	-3.44168608	-1.66564277	-1.85000546
O	-3.05794325	-0.50925704	-2.97820277
O	1.87212567	-1.77333958	-2.11865685
O	-1.56554227	4.43638751	1.97064961
O	0.15912380	3.04433929	-0.74322886
O	-2.78067604	-3.11796808	-2.24024625
O	-1.14123501	4.00773042	-2.91138300
O	-1.64507997	1.05830624	-4.61200333
Si	-0.26357004	5.47827534	1.71338709
Si	-1.76001706	-3.77082322	-3.41387806
Si	-1.45120088	5.60637732	-3.37069192
Si	-0.51466780	1.90561940	-5.54283937
Si	-0.55053050	2.50907450	4.71772076
Si	-1.78679049	-4.72495182	0.61209644
H	-0.87665685	-4.93289040	-0.55344955
H	-1.35907306	-5.58365233	1.75285009
H	-3.19614079	-5.02503417	0.23385547
H	-1.77909744	3.30494654	4.99725107
H	-0.04857868	1.86823497	5.96599299
H	0.50999400	3.37616990	4.12313768
H	0.70278698	2.18064327	-4.72569931
H	-0.16743799	1.05083489	-6.71384591
H	-1.14537026	3.17565809	-5.99750204
H	-0.91792165	6.53216182	-2.32890146
H	-0.74719459	5.81209045	-4.66685796
H	-2.92069822	5.79621502	-3.53167651
H	-0.29790910	6.49500079	2.80213609
H	1.00197519	4.69266530	1.78313737
H	-0.39561922	6.12920480	0.37703037
H	-2.13841814	-5.20327469	-3.57112617
H	-1.91796081	-3.02873723	-4.69684095
H	-0.35189673	-3.66945416	-2.92875861
Si	2.49640475	-3.31871524	-1.87463256

H	3.88328951	-3.17913177	-1.34488393
H	1.64078333	-4.06006784	-0.90268339
H	2.51346364	-4.02133240	-3.18922570
Si	3.57550052	2.53817198	1.64216422
H	2.88842451	3.21960546	2.77881317
H	3.91708157	1.13590356	2.02212915
H	4.79994639	3.28827407	1.24722503
H	-5.53731583	-1.00410632	-1.55486227
O	-5.06823891	-1.83574827	-1.73349783
H	-4.84798499	3.39486974	1.10985750
O	-4.12095244	3.83820922	1.57499701
H	-8.36999159	1.03774377	0.12409982
H	-6.19441814	2.63512303	0.53840640
H	-5.96475632	0.47729626	-1.04256604
Al	-6.77592364	1.17976101	0.15683925
N	-6.24049439	0.05878853	1.78417273
C	-6.52125893	-1.36720374	1.51287397
H	-6.27657708	-1.97283194	2.39223470
H	-7.57837252	-1.49541612	1.27321800
H	-5.91786517	-1.70535144	0.66995086
C	-7.01842251	0.50939833	2.95659862
H	-8.08248859	0.36331345	2.76749758
H	-6.72633210	-0.05909900	3.84627120
H	-6.82893412	1.56952364	3.13395352
C	-4.79520717	0.23818242	2.04454357
H	-4.47637951	-0.40317597	2.87301841
H	-4.22520996	-0.01985682	1.15226116
H	-4.60066915	1.27793384	2.30231266

B^{1}_AlH_3_NMe_3_TS_HH (N/O *cis*)

E: -1837.63768419 ; H: -1837.096402 ; G: -1837.259769

O	-0.65471405	1.22634178	3.74930164
Si	-0.73762392	0.95330696	2.14345156
O	0.65658044	1.47697579	1.42405884
Si	1.30683726	2.06226092	0.02375230
O	2.68272360	2.86183103	0.37837757
O	-0.89804791	-0.67172865	1.91393670
Si	-0.99744486	-1.63932509	0.58426252
O	-1.10367836	-3.20176931	1.04836904
O	-2.03638754	1.68873120	1.44337346
Si	-2.53474833	3.25350281	1.19014526
O	-2.37107011	3.55233726	-0.43996136
Si	-1.19653599	3.04590480	-1.48068946
O	-1.47425861	1.48027899	-1.90662796
Si	-1.30784711	0.34530386	-3.09508083
O	0.12180949	-0.44421430	-2.84468267
Si	1.13085249	-0.64517747	-1.54805377
O	1.63740071	0.82264383	-1.00921691
O	0.33972949	-1.46131244	-0.35153089
O	-2.34652873	-1.18707643	-0.24638229
Si	-3.34488148	-1.23776280	-1.55096840
O	-2.55770846	-0.72106539	-2.90806106
O	2.43445456	-1.50201733	-2.01435554
O	-1.54897882	4.23513255	2.06488476
O	0.25769745	3.11750428	-0.69219125
O	-3.88029822	-2.76923959	-1.77432420
O	-1.17184836	3.99134289	-2.81040567
O	-1.37187817	0.96359680	-4.59672051
Si	-0.43565487	5.47311149	1.78973590
Si	-3.45037998	-4.08409854	-2.74841165
Si	-1.82685909	5.47674353	-3.29161714
Si	-0.51911148	2.05734748	-5.56512214
Si	-0.34354542	2.51407657	4.79566457
Si	-2.35165568	-4.25200637	1.47990548
H	-2.74493068	-5.04791596	0.28067649
H	-1.83473566	-5.14387630	2.55320517

H	-3.52293830	-3.46233679	1.96657248
H	-1.61527241	3.23329570	5.08655034
H	0.21759733	1.92136953	6.04289908
H	0.65047551	3.43932663	4.17405755
H	0.71216508	2.50628950	-4.85384167
H	-0.16312668	1.34487001	-6.82491186
H	-1.41224009	3.21315132	-5.85800049
H	-1.60737372	6.48305686	-2.21231805
H	-1.10060478	5.86764393	-4.53171616
H	-3.28218368	5.30805493	-3.56323781
H	-0.65112090	6.50452224	2.84405813
H	0.93913086	4.90556115	1.90113926
H	-0.65052914	6.05264217	0.43136788
H	-4.22291112	-5.25282184	-2.24359834
H	-3.80178568	-3.78607310	-4.16533580
H	-1.98339455	-4.33180762	-2.61779464
Si	2.80802952	-3.07418283	-2.50020545
H	4.25226626	-3.28662626	-2.20661946
H	1.96689166	-4.04457883	-1.73959332
H	2.54715815	-3.20696224	-3.96284235
Si	3.71847568	2.95597836	1.70881985
H	3.00990450	3.62013824	2.84256078
H	4.14714502	1.58439850	2.11041737
H	4.88854673	3.76913221	1.27666756
H	-4.93475305	0.57008183	-1.90442970
O	-4.62249915	-0.23074921	-1.23562294
H	-4.76082321	3.00835588	1.16612623
O	-4.07943083	3.48362170	1.67382679
H	-7.64862597	0.25915282	-0.72180974
H	-5.86632265	2.12829080	0.45431364
H	-5.72367770	1.47216389	-2.00407649
Al	-6.17566177	0.80402723	-0.41343175
N	-5.98343191	-0.41388776	1.34385635
C	-6.15829410	-1.84115393	1.02652158
H	-6.18151079	-2.43882333	1.94587246
H	-7.09609036	-1.97988740	0.48616890
H	-5.33953886	-2.19089077	0.39880247
C	-7.07896832	0.02141709	2.22909628
H	-8.03773575	-0.13811596	1.73361240
H	-7.05946559	-0.54298851	3.16863300
H	-6.96713566	1.08404383	2.45058450
C	-4.69496961	-0.19692221	2.02664386
H	-4.64100893	-0.79111195	2.94712935
H	-3.87439204	-0.47453512	1.36909219
H	-4.59199061	0.85725146	2.28190820

B*1*_AlH3_NMe3_TS_HH (N/O *cis*) product / H2 adduct

E: -1837.70576701 ; H: -1837.162241 ; G: -1837.329608

O	-0.57651168	1.22163947	3.77108420
Si	-0.71706189	0.91392069	2.17269392
O	0.66384259	1.40018478	1.40762406
Si	1.38834762	1.87287589	-0.00023301
O	2.83865300	2.52765200	0.35940620
O	-0.94444087	-0.70342134	1.97967001
Si	-1.10684949	-1.68923074	0.66298867
O	-1.32619763	-3.22711648	1.17126665
O	-2.01254510	1.69474262	1.51443060
Si	-2.54910058	3.23984129	1.26408211
O	-2.09910783	3.70331326	-0.26941615
Si	-1.06370778	3.06948042	-1.38754844
O	-1.53451994	1.53446679	-1.74472519
Si	-1.51837765	0.37187427	-2.91932607
O	-0.16879555	-0.56156472	-2.68872505
Si	0.95959080	-0.83426163	-1.51324363
O	1.60798851	0.59122084	-1.00562327
O	0.26946808	-1.62410673	-0.23934990

O	-2.39049700	-1.14316339	-0.20179286
Si	-3.42077003	-1.45631517	-1.47179233
O	-2.85961718	-0.56266876	-2.76503345
O	2.16259629	-1.74264918	-2.13232602
O	-1.85294040	4.23692098	2.36817224
O	0.45984412	3.01270175	-0.75379053
O	-3.29163998	-3.05946441	-1.84741194
O	-1.06659952	4.01532579	-2.72042217
O	-1.50310582	1.02184253	-4.41624654
Si	-0.89158257	5.62413592	2.28741542
Si	-2.29340702	-3.96488821	-2.85769840
Si	-1.95377028	5.34597482	-3.27139067
Si	-0.39363042	1.87923639	-5.35974677
Si	0.02825794	2.47134665	4.72952325
Si	-2.60811367	-4.30330702	1.36345304
H	-2.55245538	-5.32522783	0.28049813
H	-2.45598421	-4.94850749	2.69845120
H	-3.90124423	-3.55578154	1.30203348
H	-1.11029029	3.18940742	5.36701063
H	0.90394732	1.85592618	5.76690273
H	0.82600775	3.41050904	3.88285918
H	0.82497343	2.18057454	-4.55300424
H	-0.03958292	1.02879594	-6.53225158
H	-1.04966363	3.13794958	-5.81265979
H	-1.82747216	6.46531623	-2.29359695
H	-1.36293229	5.72602345	-4.58435107
H	-3.38467599	4.95818551	-3.43227311
H	-0.63397332	6.03911236	3.69486461
H	0.39103190	5.29616546	1.59824694
H	-1.61455633	6.69751456	1.54517656
H	-2.59793555	-5.39922047	-2.59215144
H	-2.56025831	-3.62538932	-4.28540805
H	-0.86313489	-3.67929106	-2.52675582
Si	2.36125651	-3.09530595	-3.11711648
H	3.80304465	-3.14739178	-3.48800332
H	1.97443031	-4.32201878	-2.36086524
H	1.51127501	-2.95880263	-4.33632727
Si	3.58937108	3.12798486	1.74585519
H	2.87484602	4.35660143	2.20597156
H	3.56059972	2.09647862	2.82351481
H	4.99188348	3.45347641	1.36559972
H	-5.02069396	0.90058564	-3.28614570
O	-4.92862820	-1.06575263	-1.07365156
H	-4.65468447	2.76428520	0.77763807
O	-4.18210438	3.30627784	1.43063509
H	-7.42969105	0.24890108	-0.90047425
H	-5.14970214	1.65701533	-0.29995472
H	-5.56614106	1.41019431	-3.29085047
Al	-5.91253640	0.25002476	-0.41411733
N	-6.04997810	-0.31454835	1.54790848
C	-6.66912673	-1.65501246	1.60871972
H	-6.74692839	-1.99022100	2.64868136
H	-7.66550606	-1.61724376	1.16566804
H	-6.05614882	-2.35807125	1.04359474
C	-6.89401196	0.66526655	2.26127967
H	-7.86770559	0.73601252	1.77351016
H	-7.03379695	0.35920942	3.30337888
H	-6.41093008	1.64345034	2.24405632
C	-4.70508280	-0.35573369	2.16247284
H	-4.77867314	-0.64933162	3.21510914
H	-4.08561487	-1.07131196	1.62530206
H	-4.23909057	0.62638164	2.09222308

B*1*_AlH$_2$·NMe$_3$

E: -1836.52823446 ; H: -1836.001069 ; G: -1836.163084

O	-1.62896474	0.37228164	4.05340975
Si	-1.54836666	0.63359100	2.44856993
O	-0.53453949	1.89686355	2.13980063
Si	0.31407929	2.62108828	0.92315976
O	1.52436513	3.50569918	1.56116597
O	-0.99808393	-0.73530190	1.72732790
Si	-0.86227704	-1.71125757	0.40137114
O	-0.13125766	-3.10024432	0.83651412
O	-3.03756789	0.97248910	1.79505127
Si	-4.04728113	2.33088667	1.74930816
O	-3.19153671	3.59932684	1.07887783
Si	-2.30113847	3.64859056	-0.30120513
O	-2.70866883	2.29606939	-1.16709658
Si	-2.18345013	1.28297402	-2.35147333
O	-0.52963229	1.18676526	-2.29458824
Si	0.60583373	0.47133843	-1.33248395
O	0.95895713	1.46486924	-0.06565010
O	0.03653203	-0.96946828	-0.76167310
O	-2.36488804	-2.04538010	-0.19520426
Si	-3.53013319	-1.27118275	-1.06853832
O	-2.78978963	-0.21521738	-2.09188621
O	1.95953679	0.20711906	-2.20090849
O	-4.32636167	2.75572978	3.31434329
O	-0.68984611	3.60521170	0.05828890
O	-4.42477491	-2.32318291	-1.92498218
O	-2.63185411	5.01248019	-1.13483471
O	-2.62541322	1.86617078	-3.81116564
Si	-4.50955541	4.20206216	4.16031177
Si	-5.64983990	-2.22949505	-3.08917199
Si	-2.61021160	5.51320763	-2.74650453
Si	-2.00621249	1.81279386	-5.38166411
Si	-2.13448050	1.14679305	5.46686938
Si	0.08741967	-3.96473950	2.27198694
H	0.47179587	-5.34900719	1.87966643
H	1.17597411	-3.32636579	3.06692997
H	-1.18349502	-3.97205074	3.05319284
H	-3.56432178	0.81800958	5.72150534
H	-1.27163665	0.62739862	6.56476892
H	-1.95375166	2.62224539	5.32641077
H	-0.99040772	2.89404026	-5.53862945
H	-1.38477440	0.47978397	-5.63381499
H	-3.15394423	2.04031313	-6.30319451
H	-2.34692463	6.97862945	-2.74634688
H	-1.53754536	4.78261021	-3.48415347
H	-3.94011048	5.22185792	-3.35726071
H	-4.86278034	3.83288605	5.56070985
H	-3.23354459	4.97403537	4.13408887
H	-5.60676041	5.00846442	3.54603363
H	-5.91419720	-3.63224414	-3.51707290
H	-6.86927812	-1.62245322	-2.48517962
H	-5.17644249	-1.41257909	-4.24460938
O	-4.52674178	-0.51082788	0.04709252
H	-4.05009251	-0.19353590	0.83444685
Si	2.82633006	-1.14178031	-2.73217315
H	3.97110223	-0.61721546	-3.52792606
H	3.31690543	-1.91697656	-1.55617581
H	1.94900473	-1.99875390	-3.58177222
Si	3.21022642	3.52384523	1.46928353
H	3.66957375	4.60111151	2.38935067
H	3.74978809	2.20156077	1.90027364
H	3.63142706	3.81748752	0.06860091
O	-5.34348491	1.94323794	0.89897581
N	-7.13255572	2.74671652	-1.10364180
C	-6.17269975	3.79525104	-1.48624910
H	-5.58836766	4.08378933	-0.61253207
H	-5.49947758	3.40498976	-2.25128033
H	-6.69336259	4.67774513	-1.87880933

C	-7.94439728	2.36244946	-2.26725579
H	-8.52105360	3.21766459	-2.64082591
H	-7.28939060	1.99660399	-3.05962464
H	-8.63206818	1.56392066	-1.98239870
C	-8.00188561	3.22423561	-0.01803292
H	-8.69196882	2.42912586	0.26884274
H	-7.38876070	3.48225186	0.84490021
H	-8.57671395	4.10363121	-0.33529311
H	-7.30319315	0.11636815	-0.11124046
H	-5.36966973	0.91534771	-1.95844982
Al	-6.03594256	1.02187031	-0.49126326

B^{1}_AlH_2·NMe_3_TS_HH TS

E: -1836.49781053 ; H: -1835.974998 ; G: -1836.142087

O	-1.66156764	0.54379684	3.98489644
Si	-1.52908578	0.73908564	2.36942640
O	-0.35806948	1.86935717	2.06365560
Si	0.53049579	2.46200466	0.81030043
O	1.84971912	3.22046695	1.39736482
O	-1.07920305	-0.70378055	1.71604084
Si	-1.23533878	-1.62303588	0.35503705
O	-0.88205551	-3.17214855	0.73557794
O	-2.94007749	1.20866548	1.66708255
Si	-3.84851117	2.59635637	1.56697316
O	-2.92207128	3.77960067	0.82282127
Si	-1.95775461	3.65848328	-0.50389935
O	-2.42586657	2.26370186	-1.27368653
Si	-1.98682957	1.33783434	-2.56625959
O	-0.36946733	0.99286910	-2.46910805
Si	0.61257766	0.20874143	-1.39614927
O	1.02399624	1.22302547	-0.16704885
O	-0.16974216	-1.11500078	-0.79858395
O	-2.76072585	-1.52868301	-0.23619073
Si	-3.74816739	-0.94867753	-1.42544172
O	-2.86160045	-0.04825178	-2.50093870
O	1.96581581	-0.27504096	-2.16870291
O	-4.10562233	3.12569502	3.11004653
O	-0.37322620	3.53319980	-0.06489326
O	-4.39998465	-2.21647737	-2.23904833
O	-2.10288506	4.96017149	-1.47979877
O	-2.24486660	2.14371897	-3.96415492
Si	-4.20834654	4.62275411	3.86823173
Si	-3.79602820	-3.50474949	-3.14210124
Si	-3.11668003	5.43988012	-2.74099751
Si	-1.33299955	2.48032525	-5.34651482
Si	-2.09127480	1.44379796	5.34426240
Si	-0.59337851	-4.03651363	2.15433600
H	-0.54903502	-5.47512489	1.76911451
H	0.71380800	-3.61804071	2.74026679
H	-1.69297699	-3.79332779	3.13290761
H	-3.54138939	1.25047888	5.62751040
H	-1.26947584	0.92943901	6.47652099
H	-1.79547938	2.88966292	5.11642263
H	-0.22053902	3.40971891	-4.99566753
H	-0.78774868	1.21041941	-5.90822727
H	-2.26285112	3.12374336	-6.31658296
H	-3.48568043	6.86347003	-2.49544716
H	-2.36892397	5.32143933	-4.02642413
H	-4.33447281	4.57864868	-2.76357676
H	-4.58196590	4.35900208	5.28758128
H	-2.89877633	5.33377865	3.80302671
H	-5.26652304	5.45069811	3.21087152
H	-4.77934216	-4.61947932	-3.03365522
H	-3.65108000	-3.08376317	-4.56640923
H	-2.46963316	-3.92661242	-2.60060381
O	-4.94813773	-0.04914192	-0.76540627
H	-6.12688135	-0.16840507	-0.65493985

Si	2.72897088	-1.75748313	-2.43504351
H	4.00456888	-1.45241666	-3.14077540
H	3.00069579	-2.42712730	-1.12951325
H	1.85925127	-2.62468140	-3.28233039
Si	3.48926387	3.26023820	0.99674822
H	4.08995488	4.37506929	1.78096090
H	4.12519385	1.96227200	1.36541411
H	3.64520413	3.50712474	-0.46656705
O	-5.22270914	2.35328894	0.76653836
N	-7.62534633	2.88370789	-0.54881992
C	-7.20729226	4.29279719	-0.66595612
H	-6.50380160	4.52701668	0.13297053
H	-6.71468882	4.44534457	-1.62781862
H	-8.07470122	4.95969327	-0.59690474
C	-8.55248985	2.55042697	-1.64232424
H	-9.43831025	3.19543069	-1.60967266
H	-8.04755712	2.68375729	-2.60076731
H	-8.86610037	1.50938803	-1.55038463
C	-8.27671927	2.66139432	0.75395088
H	-8.55654218	1.61049084	0.84511553
H	-7.57502608	2.90797570	1.55003341
H	-9.17564516	3.28220180	0.84604462
H	-7.04276655	0.32749071	-0.55107816
H	-5.52753742	2.25138344	-2.18917281
Al	-5.88399175	1.70209814	-0.73852926

B^{1}_AlH_2·NMe_3_TS_HH product / H_2 adduct

E: -1836.56484897 ; H: -1836.039885 ; G: -1836.208143

O	-1.53798697	0.92988518	3.95402012
Si	-1.51752415	1.14216264	2.33322042
O	-0.24708980	2.12526916	1.94747227
Si	0.70623504	2.56170551	0.67673102
O	2.10329849	3.19397493	1.23112293
O	-1.30446824	-0.32783756	1.62144397
Si	-1.63590139	-1.17795504	0.24642468
O	-1.61818371	-2.77257580	0.61214595
O	-2.92141309	1.80001975	1.79565268
Si	-3.65087169	3.26228359	1.49400054
O	-2.56587036	4.23884620	0.67621249
Si	-1.64186556	3.99221895	-0.66146334
O	-2.27839245	2.64770348	-1.41385761
Si	-1.87147891	1.72448444	-2.73309935
O	-0.30495349	1.20772527	-2.57206070
Si	0.52007721	0.28420738	-1.47876372
O	1.05583925	1.23350348	-0.24377696
O	-0.46811434	-0.89770633	-0.88611310
O	-3.09805579	-0.74191462	-0.34566148
Si	-3.95610765	-0.25627967	-1.68400307
O	-2.89592659	0.44861177	-2.76363137
O	1.79598801	-0.41502676	-2.21683124
O	-3.93990533	4.01043838	2.93356131
O	-0.07738930	3.68967255	-0.23784210
O	-4.56808316	-1.59741650	-2.41859325
O	-1.63552116	5.28881610	-1.64972477
O	-1.97165659	2.61980545	-4.09622395
Si	-3.27072146	5.34334747	3.71640378
Si	-4.09951305	-3.21011598	-2.52368761
Si	-2.62023435	5.97103995	-2.84014614
Si	-0.95475298	2.97592627	-5.39955081
Si	-2.49963799	1.38781909	5.25893682
Si	-1.58561921	-3.67058368	2.03916098
H	-1.76981739	-5.09576074	1.64542529
H	-0.27196478	-3.48645568	2.72241746
H	-2.69359942	-3.23344221	2.93895475
H	-3.93084432	1.08225976	4.97040351
H	-2.02501459	0.60237654	6.43278297

H	-2.33213041	2.84873927	5.51786883
H	0.22669944	3.74481587	-4.91260917
H	-0.51528296	1.70807804	-6.05120265
H	-1.75952428	3.79878153	-6.34484239
H	-2.79626295	7.41148832	-2.49849009
H	-1.92260023	5.84135060	-4.15267458
H	-3.93471588	5.26927077	-2.87312921
H	-3.88135491	5.38595093	5.07663346
H	-1.78994994	5.18818387	3.82313743
H	-3.60031513	6.59358802	2.96992400
H	-4.54891128	-3.94451266	-1.30385650
H	-4.76061097	-3.77871433	-3.73307252
H	-2.61446475	-3.30487529	-2.65081480
O	-5.14332497	0.74746718	-1.26325552
H	-6.92410109	-1.69401921	-1.37358903
Si	2.35893137	-1.99970124	-2.37523112
H	3.63805352	-1.91738965	-3.13347412
H	2.59126134	-2.58875136	-1.02347105
H	1.35843865	-2.81577656	-3.12196568
Si	3.73010594	2.74751036	1.18672944
H	4.46079161	3.72913558	2.03640723
H	3.88910119	1.36697162	1.73052500
H	4.22752500	2.80252039	-0.21842211
O	-5.00583614	3.02455831	0.65480233
N	-7.51805027	2.13192099	-0.43262674
C	-8.10996314	3.42146674	-0.02213908
H	-7.57986236	3.79669809	0.85342840
H	-8.01177892	4.14430284	-0.83428073
H	-9.17092110	3.29169962	0.21685973
C	-8.21356134	1.61149210	-1.62801043
H	-9.27234751	1.43977804	-1.40683769
H	-8.12950015	2.33504644	-2.44090891
H	-7.74779914	0.67466815	-1.93393605
C	-7.61915493	1.15588091	0.67381952
H	-7.15275216	0.21974038	0.36868486
H	-7.09515086	1.54753994	1.54562155
H	-8.67073603	0.97914162	0.92413564
H	-7.55188991	-1.99062252	-1.09991907
H	-5.57195579	3.43790274	-2.10701107
Al	-5.56810327	2.41229686	-0.89733449

B^{1}_AlH·NMe$_3$

E: -1835.38714633 ; H: -1834.877680 ; G: -1835.042137

O	-0.94585581	0.75182696	3.39480248
Si	-0.65243145	0.88988623	1.79282571
O	0.74229851	1.75279411	1.57843382
Si	1.89147566	2.06727735	0.44046371
O	3.24017603	2.62619925	1.16730783
O	-0.46492098	-0.62320675	1.17264766
Si	-0.67934715	-1.49056096	-0.21666440
O	-0.85405859	-3.06718330	0.18283196
O	-1.88940148	1.63563991	1.01193425
Si	-2.45259807	3.13966024	0.59408906
O	-1.20481210	4.00466900	-0.10964884
Si	-0.11988724	3.61749351	-1.28254939
O	-0.76085741	2.30632383	-2.08636855
Si	-0.23796754	1.28666940	-3.28866273
O	1.24120131	0.66959581	-2.87002960
Si	1.82513720	-0.27258562	-1.64222411
O	2.26895715	0.67826750	-0.37491725
O	0.65967678	-1.34250049	-1.17392527
O	-1.99818665	-0.95679455	-1.02116877
Si	-2.61316126	-0.46207784	-2.48410577
O	-1.34716023	0.09040463	-3.42392195
O	3.13247247	-1.09942384	-2.16230846
O	-2.84187908	3.95055547	1.97536401

O	-3.71241106	2.98346108	-0.39911898
O	1.33111072	3.20022191	-0.62053441
O	-3.24490745	-1.77307259	-3.25370738
O	0.15055668	4.86544740	-2.29845979
O	-0.06233580	2.10615495	-4.69239430
Si	-2.32939118	5.39089113	2.68199460
Si	-2.70768667	-3.33570396	-3.56567331
Si	-0.66950302	5.60262098	-3.57864197
Si	1.22232360	2.43840719	-5.73963337
Si	-1.74210049	1.63085338	4.59252296
Si	-0.79867174	-3.95904515	1.61293055
H	-0.97984606	-5.38651429	1.22585578
H	0.52157434	-3.76672734	2.28181287
H	-1.89928359	-3.52432501	2.52200966
H	-3.20933113	1.63260329	4.32747976
H	-1.44579293	0.94965484	5.88409962
H	-1.22560438	3.03195643	4.61836467
H	2.26314153	3.22573520	-5.01755605
H	1.79858757	1.15844412	-6.24525325
H	0.65310380	3.23298820	-6.86390879
H	-0.70076667	7.06761942	-3.30641294
H	0.08877351	5.33178485	-4.83474433
H	-2.05203648	5.05128409	-3.67397060
H	-3.06125906	5.50969395	3.97638494
H	-0.85770101	5.35289645	2.92755619
H	-2.67043110	6.54355778	1.79596350
H	-3.45989055	-4.28920441	-2.69814475
H	-2.97803888	-3.63635727	-5.00166739
H	-1.24392932	-3.44314488	-3.28600185
O	-3.74419735	0.66222886	-2.27033283
Si	3.39677111	-2.66685025	-2.73336797
H	4.77503743	-2.68461788	-3.29734583
H	3.28120225	-3.63532680	-1.60513599
H	2.39545146	-2.99140395	-3.79186186
Si	4.85140977	2.12841713	1.25183174
H	5.57678909	3.17670177	2.02279391
H	4.93325256	0.81516942	1.95502920
H	5.41579286	2.00887708	-0.12405573
H	-4.01720538	3.34201408	-3.20445059
Al	-4.15128819	2.34289058	-1.97960297
N	-6.14025022	2.11131821	-1.67884059
C	-6.74452993	1.56103423	-2.91031254
H	-6.57348185	2.25013650	-3.73940105
H	-6.27617519	0.60380964	-3.14034302
H	-7.82197692	1.42063415	-2.77357298
C	-6.73729671	3.42436702	-1.36119722
H	-7.81598119	3.32201280	-1.20156823
H	-6.27037854	3.82205995	-0.45978004
H	-6.55947610	4.11499831	-2.18748369
C	-6.35052276	1.17540934	-0.55347897
H	-7.42172166	1.02939612	-0.37839449
H	-5.88371756	0.21961823	-0.79103446
H	-5.88437306	1.58404860	0.34300955