Supplementary information

Heterolytic cleavage of ammonia N-H bond by bifunctional activation in silica-grafted Ta(V) imido amido surface complex. Importance of the outer sphere NH_3 assistance.

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Experimental part

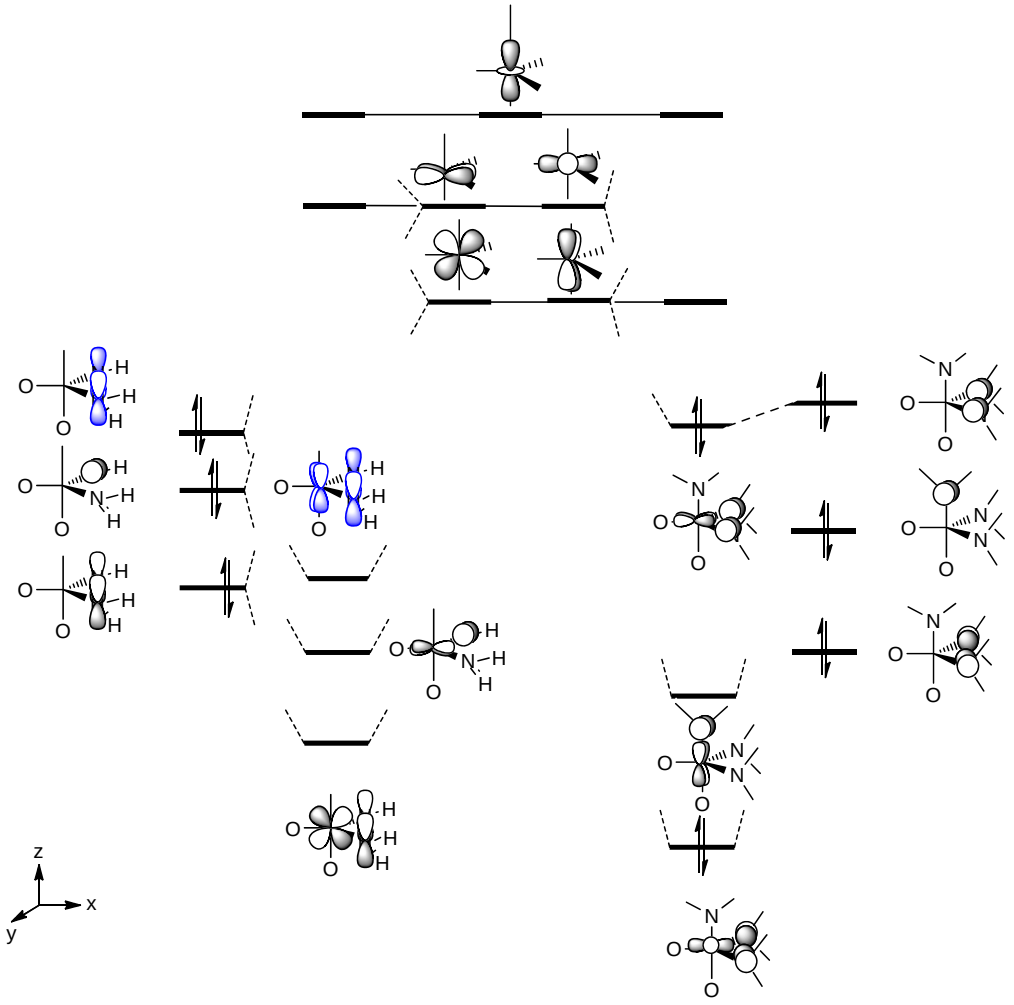
1) Reaction of [(≡SiO)Ta(=ND)(-ND_2)] with NH_3 for the *in situ* IR monitoring experiment: A large excess of deuterium (60 equivalents per tantalum) was added to a reactor containing a disk of [$(\equiv SiO)_2Ta(=NH)(-NH_2)$], **2** (15 mg, 0,012 mmol Ta) prepared as described in the experimental section, leading to the deutered species [$(\equiv SiO)_3Ta(=ND)(-ND_2)$], **2-d**, and [≡SiD] and [≡SiOD][1]

selected IR frequencies (cm^{-1}) : 2757 (ν_{OD}), 2600(ν_{SiND2}), 2580(ν_{TaND2}), 2520 ($\nu_{TaND2} + \nu_{SiND2}$), 2474 ($\nu_{TaND2}$).

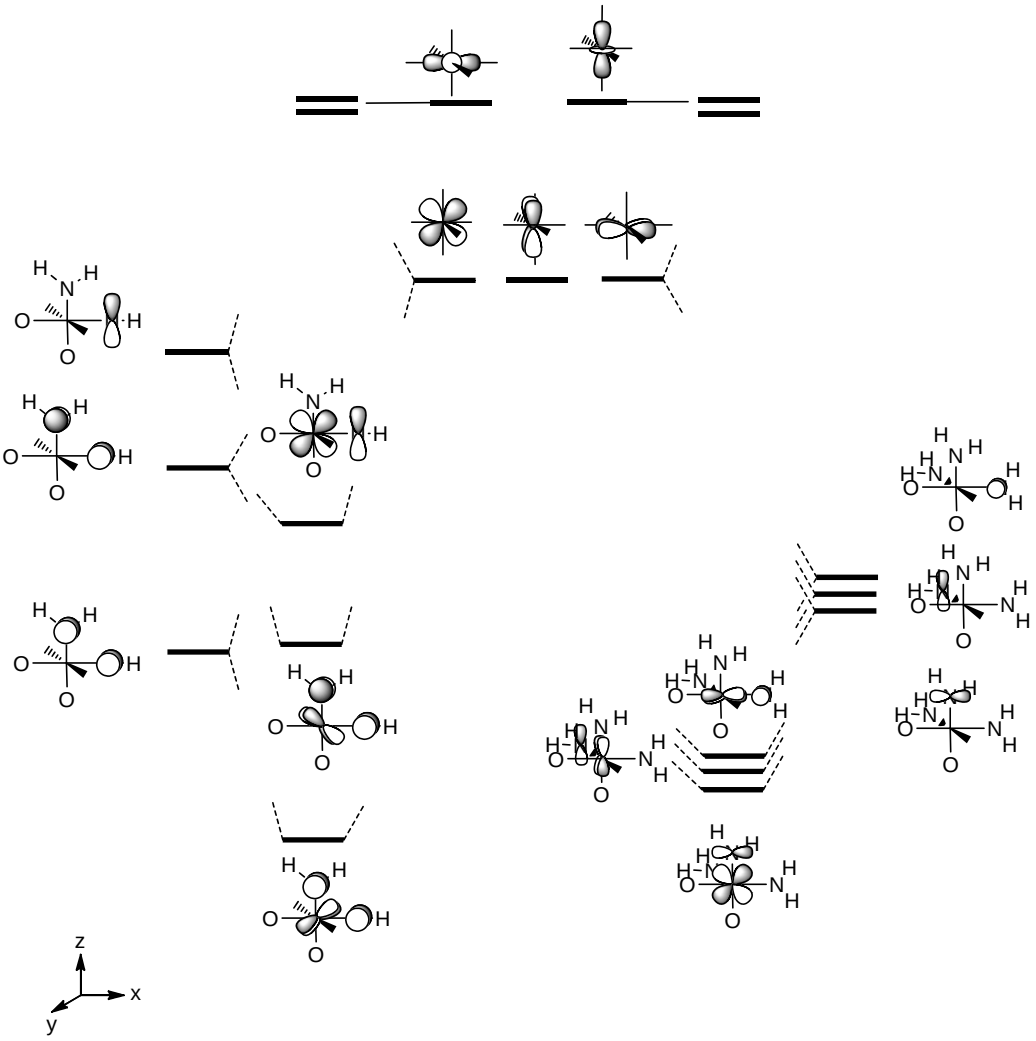
An aliquot of dry regular ammonia was added (5 torr) and the IR evolution was monitored after each addition. After a thermal treatment at 150°C during 50h, a further spectrum was acquired. Finally, a second addition of NH_3 (5 torr, 5 eq per Ta) was added a. After 10 minutes at room temperature, the spectrum was recorded while condensing the gas phase in liquid nitrogen trap.

Selected IR frequencies (cm^{-1}): 3520 (ν_{SiNH2}), 3500: (ν_{NH}), 3450 (ν_{NH}), 3378 (ν_{NH}), 3293 (ν_{NH3}), 1610 (δ_{NH3}), 1550 (δ_{SiNH2}), 1515 (δ_{NH2})

(1) P. Avenier; X. Solans-Monfort; L. Veyre; F. Renili; J. M. Basset; O. Eisenstein; M. Taoufik; E. A. Quadrelli. *Top. in Catal.* 2009, **52**, 1482.



Scheme S1



Scheme S2

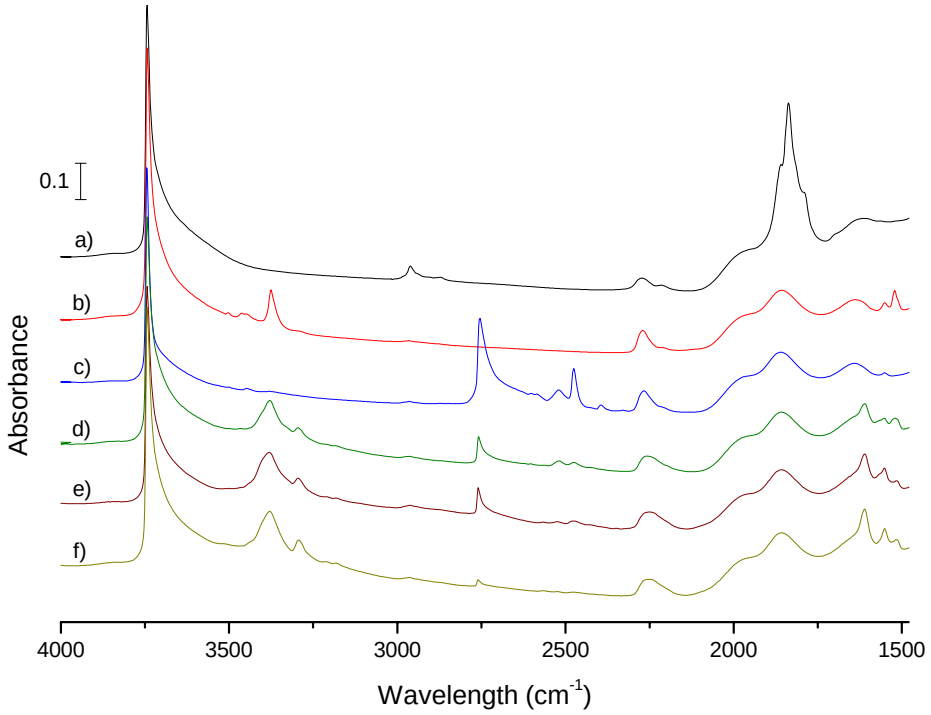
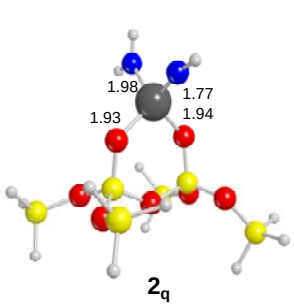
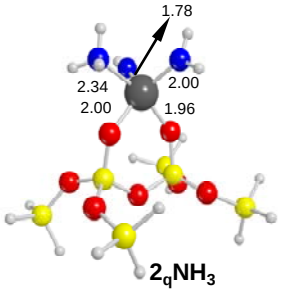


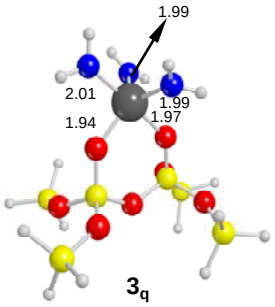
Fig. S1 IR spectra of a) tantalum hydrides [(≡SiO)$_2$Ta-H] **1a** and [(≡SiO)$_2$Ta-H$_3$] **1b** ; b) addition of N_2/H_2 (1/1) (P_{tot} = 550 torr, 250°C, 72h) ; c) addition of large excess of D_2 (P = 550 torr, 150°C, 12h) ; d) addition of dry ammonia (5 torr) ; e) thermal treatment at 150°C ; f) second addition of dry ammonia (5 torr) condensed to the sample order by cooling the reactor in liquid nitrogen.



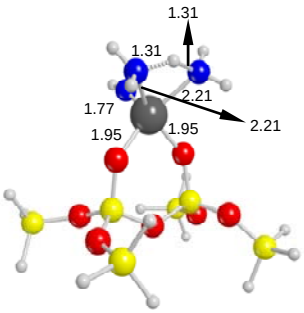
2_q



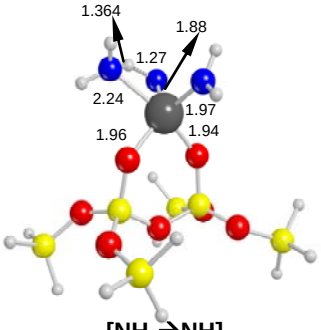
2_qNH_3



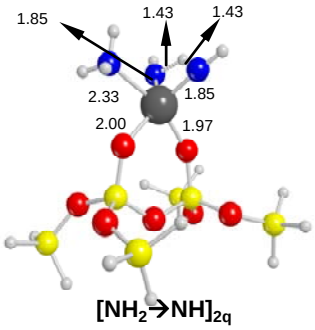
3_q



$[NH_3 \rightarrow NH_2]_{2q}$



$[NH_3 \rightarrow NH]_{2q}$



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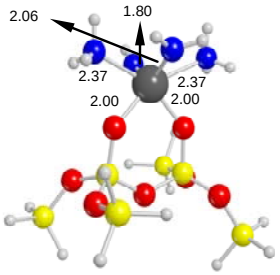
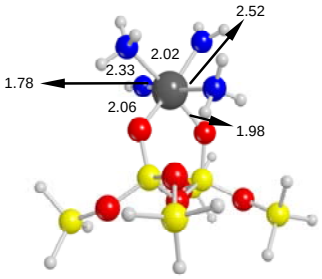
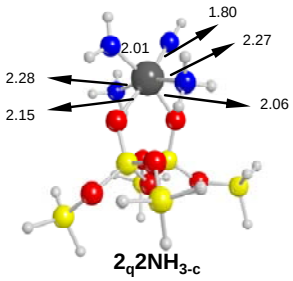


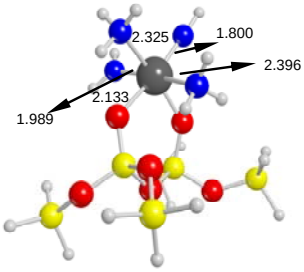
$2_q2NH_{3\text{-}a}$



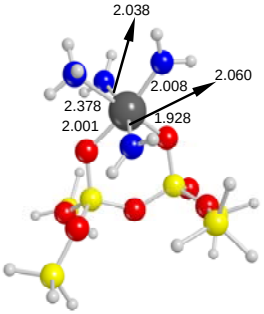
$2_q2NH_{3\text{-}b}$



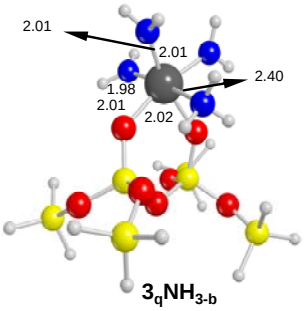
$2_q2NH_{3\text{-}c}$



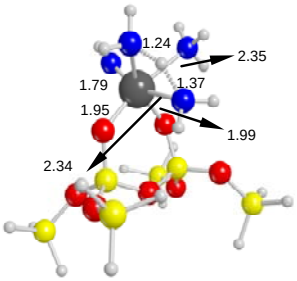
$2_q2NH_{3\text{-}d}$



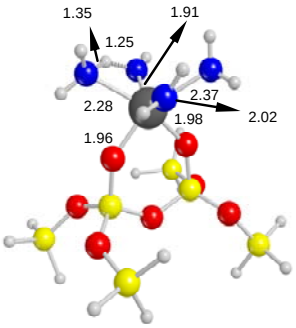
$3_qNH_{3\text{-}a}$



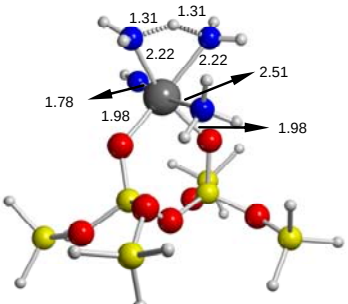
$3_qNH_{3\text{-}b}$



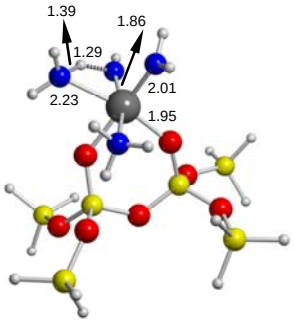
$[NH_3 \rightarrow NH_2]_{2q2NH3\text{-}a}$



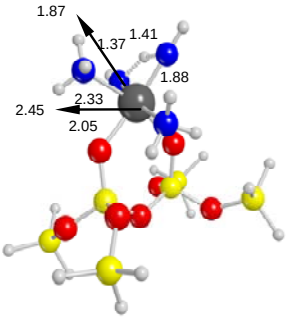
$[NH_3 \rightarrow NH]_{2q2NH3\text{-}a}$



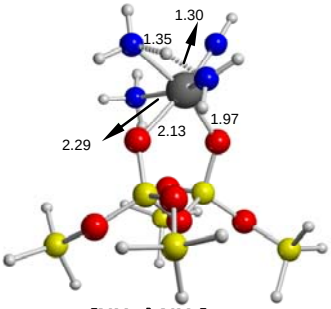
$[NH_3 \rightarrow NH_2]_{2q2NH3\text{-}b}$



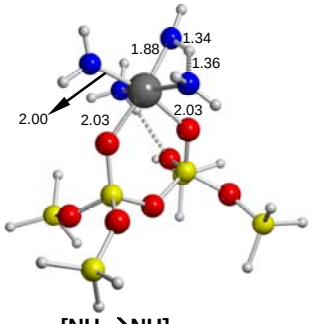
$[NH_3 \rightarrow NH]_{2q2NH3\text{-}b}$



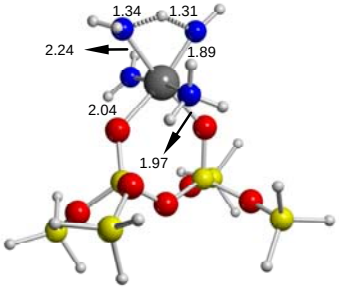
$[NH_2 \rightarrow NH]_{2q2NH3\text{-}b}$



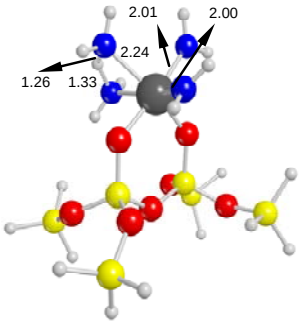
$[NH_3 \rightarrow NH_2]_{2q2NH3\text{-}c}$



$[NH_3 \rightarrow NH]_{2q2NH3\text{-}c}$



$[NH_3 \rightarrow NH]_{2q2NH3\text{-}d}$



$[NH_3 \rightarrow NH_2]_{3qNH3\text{-}a}$

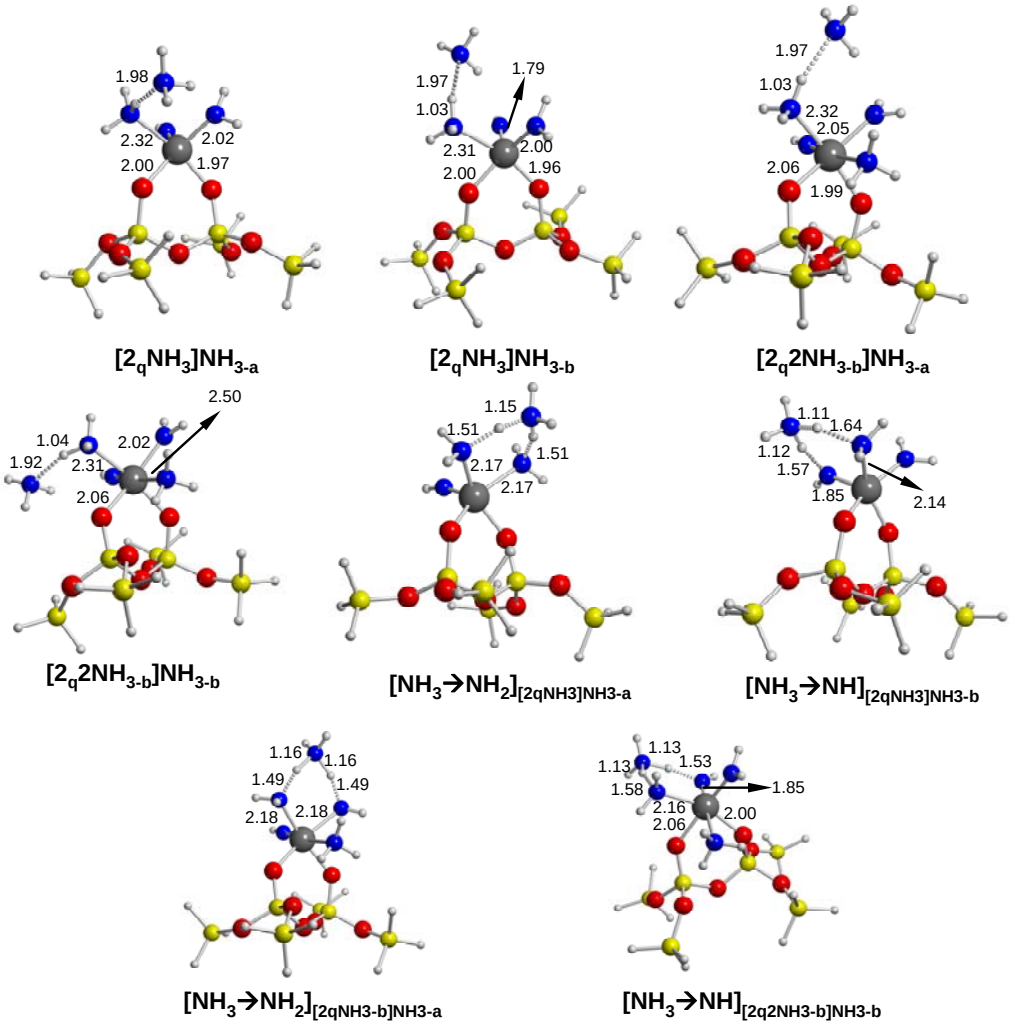


Figure S2 - DFT optimized geometries of all considered intermediates and transition states. Distances in Å

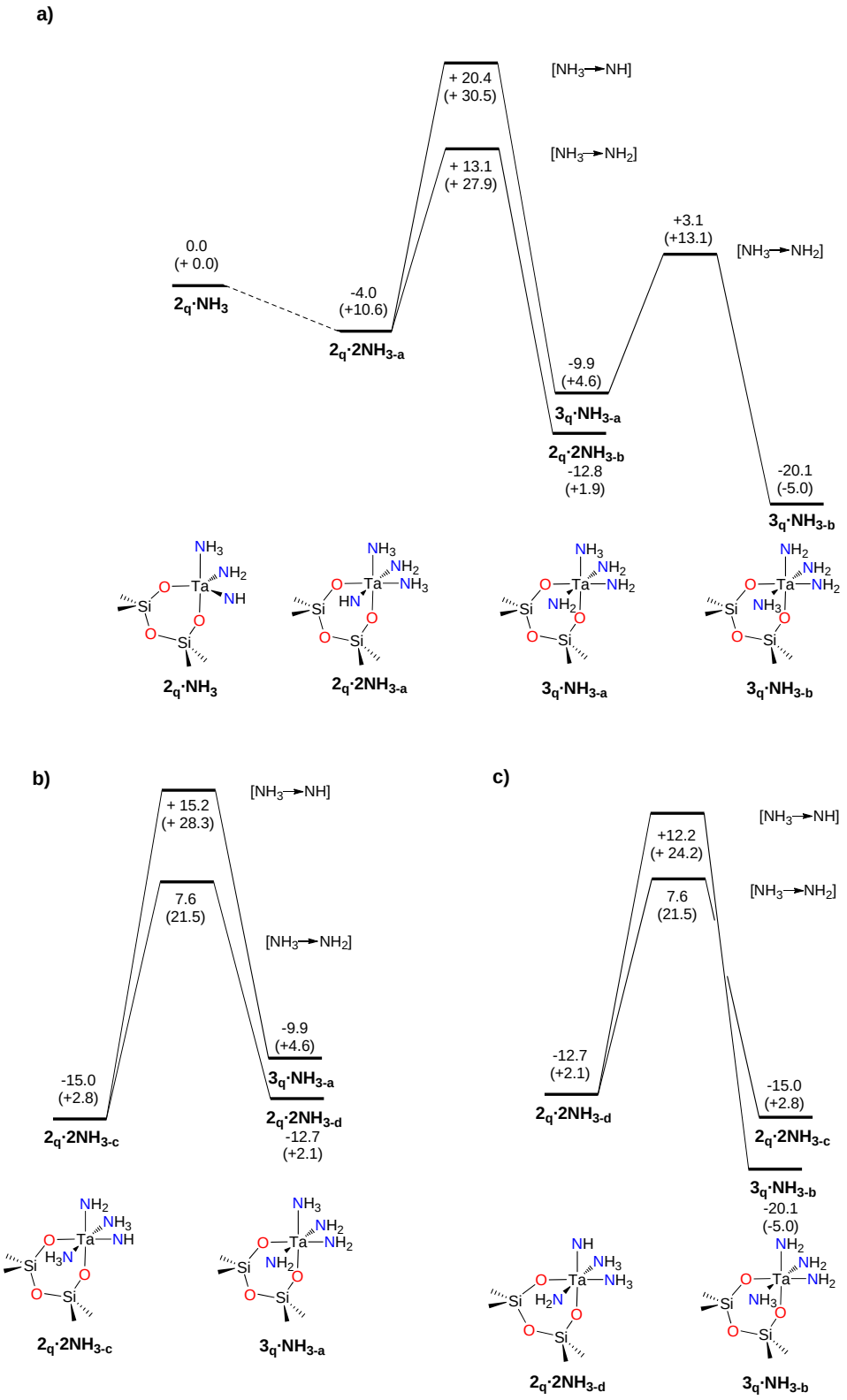


Figure S3. Computed potential energies and Gibbs free energies in parenthesis (kcal mol^{-1}) for the [NH_3→NH] and [NH_3→NH_2] H-transfer processes starting from a) **2q•2NH$_{3\text{-a}}$**, b) **2q•2NH$_{3\text{-c}}$** and c) **2q•2NH$_{3\text{-d}}$**.

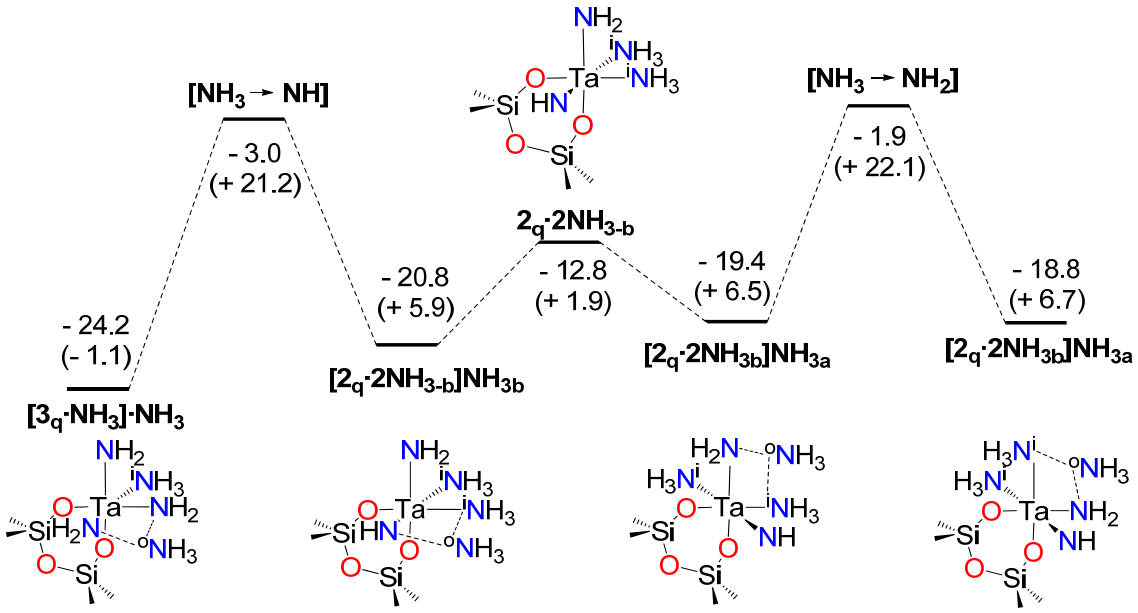


Figure S4. Computed potential energies and Gibbs free energies in parenthesis (kcal mol^{-1}) for the outer sphere assisted H-transfer paths for **2q•2NH$_3$**: i) from coordinated ammonia to imido ligand [$NH_3 \rightarrow NH$], and ii) from coordinated ammonia to amido ligand, [$NH_3 \rightarrow NH_2$]

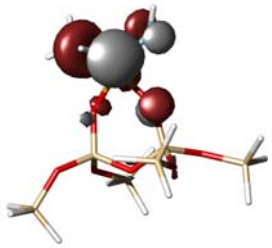
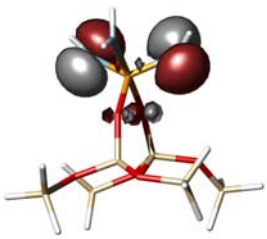
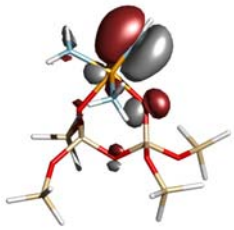
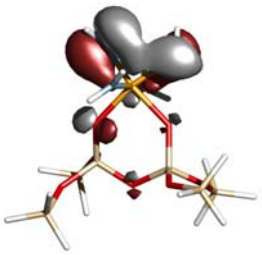
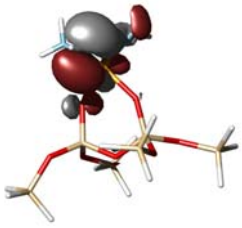
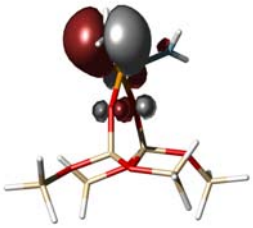
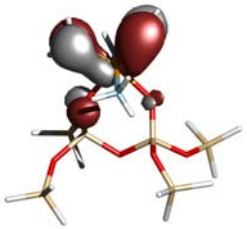
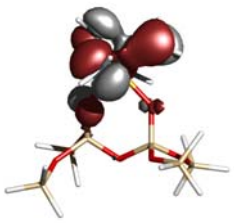
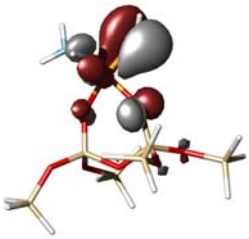
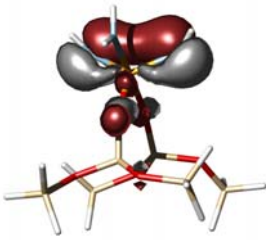
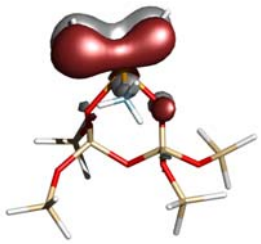
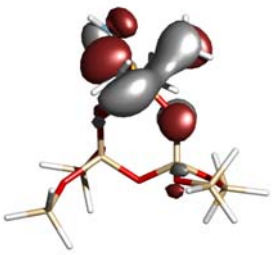
2q·NH$_3$	**3q**	**2q·2NH$_{3c}$**	**3q·NH$_{3c}$**
HOMO	HOMO	HOMO	HOMO
			
-0.25818	-0.25566	-0.24235	-0.25478
HOMO-1	HOMO-1	HOMO-1	HOMO-1
			
-0.26516	-0.28557	-0.25127	-0.26229
HOMO-2	HOMO-2	HOMO-2	HOMO-2
			
-0.26843	-0.28408	-0.26063	-0.26716

Figure S5. Kohn-Sham orbitals responsible of the d_π/p_π interactions in the lower in energy isomers of **2$_q$·NH$_3$**, **3$_q$**, **2$_q$·2NH$_3$** and **3$_q$·NH$_3$**

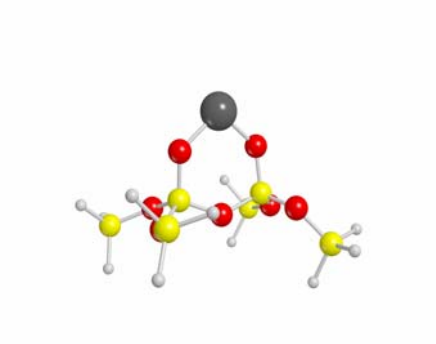


Figure S6. Computational model

Optimized Cartesian coordinates.

2_q

O	-2.889253	0.577453	-1.200163
O	-2.663624	0.173063	1.430404
O	-0.646786	1.373028	0.092295
O	-1.120892	-1.263974	-0.245476
Si	-1.833141	0.210533	0.012998
H	1.287008	-2.573286	-2.588210
N	1.317942	-2.915603	-1.632407
Ta	0.706275	-1.870404	-0.066972
H	1.704268	-3.851918	-1.609661
O	1.591580	2.287979	1.321385
O	1.463960	2.138289	-1.343151
O	1.591098	-0.155041	0.106607
Si	1.011979	1.400792	0.058612
N	0.984171	-2.928263	1.331410
H	1.042083	-3.376150	2.236626
Si	-2.741007	1.100045	-2.799668
H	-1.573436	0.431570	-3.452661
H	-4.004966	0.718313	-3.492265
H	-2.558917	2.581127	-2.829748
Si	2.661447	3.266533	-1.729113
H	3.985874	2.821868	-1.198737
H	2.701448	3.332520	-3.218815
H	2.308203	4.602270	-1.163056
Si	1.910823	1.968034	2.951514
H	3.277044	1.380295	3.082158
H	1.842913	3.277350	3.661702
H	0.892482	1.023377	3.501377
Si	-4.123014	0.837540	1.961378
H	-5.269919	0.122139	1.326685
H	-4.152304	0.649621	3.440426
H	-4.182530	2.292412	1.624816

E = -726.084779333
G = -725.981084

$2_q \cdot NH_3$

O	-1.885587	-2.334493	-1.183241
O	-1.376375	-2.352443	1.430941
O	-1.753745	0.008996	0.151086
O	0.513504	-1.440521	-0.248014
Si	-1.101867	-1.516957	0.031155
H	2.845421	0.948551	-2.397200
N	3.153772	0.715898	-1.458254
Ta	1.983592	-0.096554	-0.055298
H	4.081522	1.092354	-1.302982
H	2.779995	-2.459471	-1.518534
H	4.042215	-2.049527	-0.546154
N	3.028904	-2.117223	-0.592971
H	2.726347	-2.823486	0.074823
O	-1.541418	2.453954	1.298690
O	-1.515029	2.200971	-1.350239
O	0.617773	1.303088	0.083489
Si	-1.011802	1.493791	0.057916
N	2.919357	-0.018451	1.457534
H	3.200531	-0.009110	2.429394
Si	-2.541979	-1.848076	-2.658263
H	-1.574489	-0.979296	-3.398018
H	-2.796784	-3.095471	-3.438060
H	-3.821453	-1.109873	-2.442706
Si	-2.055260	3.755532	-1.714343
H	-1.082517	4.781659	-1.227968
H	-2.157992	3.823040	-3.202381
H	-3.395291	4.000984	-1.101265
Si	-1.030498	2.690078	2.889568
H	0.182924	3.561006	2.912942
H	-2.155554	3.366996	3.598719
H	-0.726825	1.380889	3.543914
Si	-2.685044	-3.258845	1.983980
H	-2.632379	-4.635743	1.403938
H	-2.556606	-3.332950	3.469240
H	-3.978172	-2.607399	1.613018

E = -782.662086419
G = -782.520193

$[NH_3\text{-}NH_2]_{2q}$

O	-0.141547	2.972078	-1.230624
O	-0.326617	2.637981	1.404266
O	1.373392	1.103681	0.028201
O	-1.279536	0.702067	-0.267591
Si	-0.112434	1.842941	-0.022663
H	-0.796190	-3.392087	-1.633294
N	-1.577183	-3.139208	-1.033010
Ta	-1.476166	-1.216337	0.048290
H	-1.830829	-3.959939	-0.490216
H	-3.073802	-0.631914	-2.219635
H	-2.555315	-2.442765	-1.538849
N	-3.117673	-1.269787	-1.429017
H	-4.065932	-1.249700	-1.064586
O	2.892198	-0.731561	1.312143
O	2.566386	-0.900435	-1.320976
O	0.454424	-1.425656	0.265326
Si	1.806381	-0.500390	0.090456
N	-2.310937	-1.564208	1.572112
H	-2.609607	-1.583491	2.538555
Si	0.220525	2.987674	-2.875697
H	-0.466533	4.177418	-3.456727
H	1.696564	3.096353	-3.072825
H	-0.282084	1.739654	-3.531685
Si	-1.224854	3.981181	1.884665
H	-2.603064	3.925213	1.307373
H	-1.292680	3.935137	3.374359
H	-0.544450	5.235211	1.441870
Si	4.192122	-1.080877	-1.737649
H	4.758157	-2.304155	-1.093043
H	4.224670	-1.228606	-3.222590
H	4.978711	0.120522	-1.325186
Si	2.857978	-0.646178	2.998428
H	4.244694	-0.317340	3.439375
H	1.904248	0.411506	3.448431
H	2.448434	-1.972160	3.551424

E = -782.630241311
G = -782.492707

$[NH_2\text{-}NH]_{2qNH3}$

O	-2.512251	-1.684537	-1.211072

O	-2.130161	-1.729942	1.428005
O	-1.715411	0.568656	0.035285
O	0.006015	-1.530149	-0.170554
Si	-1.564902	-1.086280	0.012281
H	3.737739	-0.160575	-2.112133
N	3.083580	-0.414446	-1.388561
Ta	1.831794	-0.718397	-0.061456
H	3.654150	-0.419982	-0.078202
H	1.686933	-3.359348	-1.124993
H	3.136174	-3.273760	-0.343517
N	2.154147	-3.017191	-0.287601
H	1.741236	-3.516232	0.497945
O	-0.790398	2.786661	1.293361
O	-0.695506	2.578656	-1.364596
O	0.947272	1.021438	0.176186
Si	-0.525171	1.731299	0.043583
N	3.150089	-0.682069	1.237723
H	3.851925	-0.619755	1.958515
Si	-3.018818	-1.033291	-2.683959
H	-1.866016	-0.415643	-3.407901
H	-3.563950	-2.174080	-3.478229
H	-4.085611	-0.013024	-2.460317
Si	-0.420449	4.187566	-1.781065
H	0.863948	4.677394	-1.192096
H	-0.344736	4.233460	-3.271252
H	-1.548999	5.043183	-1.304470
Si	-0.218930	2.847287	2.879047
H	1.166951	3.405055	2.904157
H	-1.141048	3.749618	3.629173
H	-0.225799	1.484930	3.494942
Si	-3.680721	-2.128097	1.956406
H	-4.678067	-1.119360	1.485973
H	-4.057847	-3.482649	1.448474
H	-3.633279	-2.145337	3.448285

E = -782.588988192
G = -782.451138

$[NH_3 \rightarrow NH]_{2q \cdot NH3}$

O	1.632701	2.360573	-1.398792
O	1.219904	2.475501	1.231103
O	1.735278	0.091125	0.082349
O	-0.642931	1.305156	-0.326819
Si	0.971204	1.557142	-0.114646
H	-2.663662	-0.762698	-2.554618
N	-2.993336	-0.799106	-1.594784
Ta	-1.972535	-0.107997	-0.057136
H	-3.891933	-1.266542	-1.553285
H	-2.962938	2.496445	0.578679
H	-4.139449	1.773149	-0.317402
N	-3.373803	1.602078	0.327577
H	-3.466989	0.629754	1.279510
O	1.687826	-2.259797	1.447132
O	1.676551	-2.247491	-1.220273
O	-0.520194	-1.380861	0.101292
Si	1.131874	-1.454924	0.117574
N	-2.931954	-0.493397	1.514769
H	-2.900177	-0.989337	2.397142
Si	2.089863	1.934950	-2.966739
H	1.071335	1.022394	-3.572381
H	2.167037	3.203629	-3.747185
H	3.421592	1.261035	-2.942821
Si	2.219609	-3.817873	-1.516271
H	1.232073	-4.816757	-1.005747
H	2.351302	-3.939376	-2.997502
H	3.545517	-4.035989	-0.864188
Si	1.875822	-1.883672	3.082923
H	1.948891	-3.182593	3.812093
H	3.137895	-1.110398	3.278668
H	0.709527	-1.083940	3.566889
Si	2.253417	3.762247	1.585130
H	1.805979	4.993561	0.867104
H	2.167998	3.971393	3.059801
H	3.656582	3.429220	1.193735

E = -782.618037131
G = -782.482842

3_q

O	0.421565	2.649566	-1.287714
O	0.515057	2.777858	1.372892
O	1.562275	0.638889	0.067747
O	-1.119899	0.965449	0.172529
Si	0.332452	1.751778	0.091376
H	-1.747399	-2.268148	-2.266396
N	-2.343624	-1.626746	-1.755892
Ta	-1.835423	-0.828727	-0.006873
H	-3.218173	-1.473227	-2.241177
H	-3.835014	0.944024	0.439780
H	-4.543499	-0.544074	0.294839
N	-3.659702	-0.042851	0.276669
O	2.208305	-1.707152	1.246424
O	2.501566	-1.445458	-1.385455
O	-0.006320	-1.516860	-0.275860
Si	1.550294	-1.019301	-0.101777
N	-1.995533	-2.028225	1.567977
H	-1.298507	-2.726766	1.799426
H	-2.761115	-2.035262	2.229410
Si	0.213005	4.286246	-1.637720
H	-1.083231	4.778405	-1.078573
H	1.341981	5.084108	-1.071746
H	0.203017	4.397963	-3.125350
Si	0.939952	2.599212	2.997351
H	0.459013	3.825420	3.697735
H	0.287508	1.384912	3.574519
H	2.423870	2.486329	3.120722
Si	2.775138	-0.833781	-2.935014
H	3.477307	-1.909682	-3.693524
H	1.478293	-0.500064	-3.598775
H	3.634890	0.384448	-2.857312
Si	3.754669	-2.283252	1.600359
H	3.791495	-2.500654	3.076225
H	3.998267	-3.573953	0.888489
H	4.791650	-1.282913	1.203600

E = -782.670231656
G = -782.530270

$2_q \cdot 2NH_{3\text{-}a}$

O	1.745051	2.495643	-1.065685

O	1.549646	2.212641	1.557162
O	1.876902	0.020584	0.013119
O	-0.489010	1.353343	0.011134
Si	1.133148	1.503672	0.120439
H	-3.470365	1.050210	-2.018266
N	-3.136076	0.176917	-1.627709
Ta	-1.936551	-0.031438	0.034007
H	-3.432156	-0.569721	-2.245889
H	-2.698968	2.749373	-0.501639
H	-3.947188	2.086956	0.360737
N	-2.937230	2.104516	0.248856
H	-2.530969	2.479441	1.101930
O	1.666848	-2.461284	1.053743
O	1.741817	-2.168044	-1.573314
O	-0.455403	-1.339604	-0.279648
Si	1.169276	-1.471545	-0.184446
N	-2.527881	-0.252565	1.720336
H	-3.013574	-0.354619	2.601831
N	-2.890080	-2.165952	-0.322724
H	-3.902749	-2.193316	-0.241544
H	-2.617834	-2.590122	-1.207055
H	-2.497130	-2.742884	0.415986
Si	1.598000	2.562451	-2.739142
H	0.317643	3.244825	-3.108934
H	2.750423	3.363173	-3.247744
H	1.618444	1.192583	-3.336271
Si	3.111435	-3.088262	-1.903544
H	2.920671	-4.492253	-1.425033
H	3.277944	-3.085786	-3.387731
H	4.323379	-2.499591	-1.255618
Si	1.495996	-2.477176	2.727608
H	0.239117	-3.201051	3.094609
H	2.670765	-3.216105	3.278986
H	1.455659	-1.089384	3.277886
Si	2.882339	3.118097	2.042237
H	2.749756	4.528697	1.563293
H	2.893609	3.097615	3.535391
H	4.151095	2.528947	1.515028

E = -839.218065899
G = -839.037846

$2_q \cdot 2NH_{3\text{-}b}$

O	-2.116351	-1.556309	-1.102499
O	-2.560511	-1.530240	1.507231
O	-1.689145	0.714141	0.297405
O	0.012081	-1.413353	0.523266
Si	-1.531064	-0.942269	0.347440
H	-0.204781	-1.528467	-2.132117
N	0.760084	-1.231449	-2.293612
Ta	1.807597	-0.610859	-0.087554
H	0.705423	-0.333178	-2.771082
H	1.945600	-3.470155	-0.646974
H	3.172262	-3.078489	0.375112
N	2.197349	-2.895996	0.153528
H	1.619143	-3.196887	0.935920
O	-0.240668	2.664913	1.403274
O	-1.033959	2.921897	-1.122387
O	0.856027	1.067850	-0.552033
Si	-0.484047	1.828294	0.001642
N	2.681324	-0.254541	1.424257
H	3.122407	-0.010145	2.301131
N	3.387487	-0.560802	-1.348519
H	4.322459	-0.316795	-1.044374
H	3.392616	-0.711052	-2.350781
H	1.178260	-1.888714	-2.947346
Si	-3.672536	-2.072376	-1.510431
H	-3.685380	-2.202415	-2.999553
H	-3.956022	-3.403346	-0.892966
H	-4.696551	-1.076841	-1.075802
Si	-2.622400	-1.423069	3.188912
H	-2.228705	-0.058487	3.649564
H	-4.030933	-1.718921	3.584858
H	-1.709442	-2.443936	3.790395
Si	0.556284	4.085695	1.819376
H	1.812643	4.249182	1.025468
H	-0.340223	5.258211	1.580176
H	0.881815	3.993131	3.273601
Si	-1.936733	2.799147	-2.531057
H	-1.801071	4.096608	-3.255453
H	-1.417266	1.690572	-3.397200
H	-3.373424	2.535281	-2.217081

E = -839.232042364
G = -839.051701

$2_q \cdot 2NH_{3\text{-}c}$

O	0.999163	2.264594	-1.195782
O	1.799222	2.420507	1.326051
O	1.844145	0.030665	0.097717
O	-0.574942	1.165296	0.679381
Si	0.972843	1.441587	0.270381
H	-0.854121	1.680180	-1.920072
N	-1.698754	1.106319	-2.014794
Ta	-2.050113	-0.048698	-0.080192
H	-1.541405	0.450992	-2.777264
H	-2.503100	-1.817466	2.070021
H	-0.864901	-1.710479	1.834485
N	-1.740215	-1.175438	1.871879
H	-1.673507	-0.518532	2.646116
O	0.988988	-2.287762	1.223279
O	2.121727	-2.324830	-1.168171
O	-0.400000	-1.210217	-0.815374
Si	1.083782	-1.429342	-0.225669
N	-3.516199	0.844320	0.455555
H	-4.344784	1.341049	0.761831
N	-3.030306	-1.546437	-0.986442
H	-4.033501	-1.658883	-1.071563
H	-2.540012	-2.312191	-1.438243
H	-2.476066	1.710796	-2.265398
Si	2.058056	3.462309	-1.747118
H	1.765711	3.624745	-3.203931
H	1.801956	4.752133	-1.038836
H	3.478391	3.043496	-1.555800
Si	1.904311	2.503432	3.003369
H	1.366262	1.256322	3.631145
H	3.343527	2.669933	3.363523
H	1.123380	3.681854	3.487343

Si	2.098026	-3.369187	1.899732
H	2.083029	-4.666218	1.159348
H	3.475423	-2.791910	1.896999
H	1.644707	-3.592392	3.307054
Si	3.037045	-1.967079	-2.534678
H	3.329832	-3.264595	-3.212817
H	2.276582	-1.073356	-3.463511
H	4.315819	-1.301986	-2.140866

E = -839.235679181
G = -839.047695

$2_q2NH_{3\text{-}d}$

O	2.344142	-1.125269	1.308337
O	3.190966	-0.552115	-1.135897
O	1.501210	1.143652	0.093296
O	0.558522	-1.293558	-0.682938
Si	1.847992	-0.469439	-0.161817
H	0.439980	-1.693051	1.987594
N	-0.583349	-1.654395	1.991399
Ta	-1.505626	-1.156166	-0.162993
H	-0.845660	-0.845152	2.552198
H	-1.299263	-4.058911	0.338011
H	-1.602764	-3.733739	-1.239213
N	-1.076458	-3.426497	-0.424891
H	-0.082595	-3.491178	-0.644807
O	-0.218456	2.635785	-1.269412
O	-0.020105	2.950126	1.387450
O	-1.176150	0.704806	0.442894
Si	-0.012303	1.828189	0.159122
N	-1.884447	-1.012093	-2.110248
H	-1.155002	-0.829131	-2.792198
N	-3.171960	-1.486731	0.432781
H	-4.068444	-1.749765	0.824959
H	-0.941084	-2.469714	2.480884
Si	3.866201	-1.088190	2.042340
H	3.641097	-1.441756	3.477726
H	4.766109	-2.103277	1.416179
H	4.477187	0.270607	1.942996
Si	3.635624	0.243230	-2.554606
H	4.144995	1.611924	-2.242458
H	4.722087	-0.572667	-3.174553
H	2.474595	0.336140	-3.492209
Si	-1.238537	3.868314	-1.788590
H	-2.600456	3.727926	-1.186646
H	-0.662498	5.196094	-1.414778
H	-1.328194	3.759654	-3.275080
Si	-0.740358	2.912019	2.905060
H	-2.209296	3.165097	2.803649
H	-0.517021	1.586242	3.569866
H	-0.094366	3.981684	3.720752
H	-2.796908	-1.014041	-2.548643

E = -839.231925911
G = -839.051350

$3_q{\cdot}NH_{3\text{-}a}$

O	-2.021446	-2.198912	-1.332264
O	-1.416676	-2.306419	1.243599
O	-1.662187	0.103571	0.001520
O	0.454812	-1.485603	-0.606477
Si	-1.135479	-1.465165	-0.150555
H	1.958863	1.089039	-2.667504
N	2.372653	0.320991	-2.151522
Ta	1.842765	-0.195647	-0.252654
H	3.074606	-0.142562	-2.717090
H	3.105632	-2.542290	-0.138426
H	4.278150	-1.450438	0.247016
N	3.303300	-1.552791	-0.010684
O	-0.998573	2.216656	1.572803
O	-1.723598	2.624098	-0.943798
O	0.678431	1.426606	-0.386369
Si	-0.894940	1.580940	0.043125
N	1.465042	0.022813	1.760500
H	0.960075	0.787455	2.196324
N	3.556648	1.365454	0.277542
H	3.914935	1.278796	1.225391
H	4.327309	1.395987	-0.385330
H	3.075697	2.261911	0.218830
H	1.857707	-0.579184	2.476190
Si	-3.339675	-3.246947	-1.296774
H	-2.917163	-4.599042	-0.819872
H	-4.415545	-2.713963	-0.405869
H	-3.840886	-3.339581	-2.699500
Si	-1.092169	-2.184477	2.890849
H	-2.075658	-3.081566	3.569515
H	0.291615	-2.667220	3.182815
H	-1.266243	-0.783739	3.373508
Si	-2.392329	2.507120	-2.487700
H	-2.643658	3.905129	-2.946673
H	-1.442248	1.827078	-3.420310
H	-3.678438	1.749798	-2.434239
Si	-2.092780	3.301986	2.259809
H	-1.826022	3.287010	3.729046
H	-1.865936	4.677113	1.720736
H	-3.500997	2.878868	1.993657

E = -839.227520327
G = -839.047403

$3_q{\cdot}NH_{3\text{-}b}$

O	-0.281740	2.696907	1.190928
O	-0.870547	2.819267	-1.402387
O	-1.712981	0.730557	0.089456
O	0.915102	0.957022	-0.559449
Si	-0.442294	1.781012	-0.176639
H	1.737945	-0.768253	2.699752
N	2.340620	-0.533401	1.918212
Ta	1.796729	-0.767011	0.030590
H	3.212887	-0.132291	2.240796
H	3.407716	1.099851	-1.073126
H	4.275105	-0.323851	-1.017816
N	3.391470	0.122576	-0.800470
O	-2.035791	-1.706914	-1.040438
O	-2.659286	-1.359092	1.517922
O	-0.028743	-1.311149	0.683236
Si	-1.572195	-0.906874	0.355038
N	2.606100	-2.595227	-0.200808
H	3.076704	-3.052860	0.572371

N	0.893776	-1.375569	-2.105827
H	0.772528	-0.501416	-2.613580
H	1.451667	-1.990950	-2.691078
H	-0.034243	-1.790373	-1.997505
H	2.617891	-3.212431	-1.003390
Si	0.457171	4.159041	1.565276
H	1.782664	4.276560	0.881098
H	-0.417166	5.299171	1.153215
H	0.649667	4.180910	3.045658
Si	-1.673337	2.619677	-2.863166
H	-1.397093	3.834002	-3.685410
H	-1.162438	1.406672	-3.582268
H	-3.143293	2.471843	-2.643385
Si	-3.091036	-0.755427	3.033816
H	-3.865628	-1.835667	3.712132
H	-1.870101	-0.424477	3.830292
H	-3.939880	0.463000	2.877615
Si	-3.517538	-2.405491	-1.459284
H	-3.403773	-2.762367	-2.905920
H	-3.759652	-3.638976	-0.653219
H	-4.635419	-1.434902	-1.261793

E = -839.243676549
G = -839.062833

$[NH_3 \rightarrow NH_2]_{2q \cdot 2NH3\text{-}a}$

O	2.272845	-2.097540	1.067980
O	2.426614	-1.211725	-1.426822
O	1.538836	0.436201	0.533837
O	-0.017880	-1.591187	-0.354843
Si	1.531167	-1.121652	-0.044669
H	-0.839623	-0.779981	2.374702
N	-1.685967	-0.463001	1.906168
Ta	-1.693291	-0.597151	-0.429636
H	-1.958282	0.382742	2.400579
H	-2.401068	-3.100958	0.625695
H	-2.523738	-1.496652	1.584869
N	-2.862866	-2.193690	0.623495
H	-3.836297	-2.356554	0.384218
O	1.307752	2.842408	-0.686800
O	0.194188	2.451634	1.695017
O	-0.853573	1.202439	-0.501556
Si	0.517388	1.718307	0.243464
N	-2.360065	-0.835829	-2.076274
H	-2.843498	-0.982079	-2.954186
N	-3.583394	0.676831	0.136391
H	-4.029826	0.447452	1.021082
H	-3.239074	1.634062	0.201126
H	-4.284497	0.649291	-0.599168
Si	2.043455	-2.603292	2.653504
H	1.412684	-3.958167	2.651882
H	3.382262	-2.665734	3.308263
H	1.161129	-1.647574	3.394062
Si	0.906260	3.786598	2.441150
H	0.490549	5.047717	1.754446
H	0.401276	3.794206	3.847020
H	2.395494	3.671035	2.433688
Si	1.214148	3.245044	-2.322960
H	-0.089205	3.918647	-2.612700
H	2.336146	4.194583	-2.582629
H	1.357939	2.031072	-3.179950
Si	3.937028	-1.855794	-1.801948
H	3.915623	-3.344649	-1.670858
H	4.216764	-1.474956	-3.217302
H	4.989020	-1.288463	-0.903940

E = -839.190776667
G = -839.010213

$[NH_3 \rightarrow NH]_{2q \cdot 2NH3\text{-}a}$

O	-1.884358	-2.290296	-1.225086
O	-1.636959	-2.216259	1.424567
O	-1.832516	0.100508	0.044360
O	0.425264	-1.384061	-0.092144
Si	-1.210742	-1.443448	0.030396
H	2.400007	-1.261163	-2.440040
N	2.652944	-0.397827	-1.963917
Ta	1.935672	-0.141317	-0.092610
H	3.494301	-0.037146	-2.398934
H	2.411207	-2.855525	0.697981
H	3.785586	-2.383399	-0.078655
N	3.011839	-2.061369	0.495546
O	-1.463770	2.433207	1.376237
O	-1.518817	2.436225	-1.273011
O	0.588414	1.307035	-0.049857
Si	-1.031763	1.557212	0.038927
N	2.838462	0.091326	1.574879
H	3.118064	0.738503	2.301152
N	3.108009	1.858171	-0.571192
H	2.825886	2.522262	0.145207
H	4.122158	1.789896	-0.542190
H	2.829569	2.244826	-1.470760
H	3.189928	-1.100217	1.420095
Si	-2.425293	-1.866721	-2.765233
H	-2.569916	-3.140712	-3.528883
H	-3.745889	-1.174884	-2.673845
H	-1.434157	-0.975205	-3.441908
Si	-2.797120	-3.386278	1.779571
H	-2.414128	-4.697928	1.174367
H	-2.833188	-3.504010	3.266723
H	-4.139227	-2.970286	1.268849
Si	-2.735961	3.580261	-1.498163
H	-2.325188	4.891305	-0.908743
H	-2.909982	3.725090	-2.973656
H	-4.015482	3.126348	-0.873661
Si	-1.356096	2.223795	3.046184
H	-2.485781	2.987329	3.652693
H	-1.451017	0.777693	3.404407
H	-0.055987	2.782885	3.529035

E = -839.179250827
G = -839.006096

$[NH_3 \rightarrow NH_2]_{2q \cdot 2NH3\text{-}b}$

O	-2.356607	-1.221524	-1.072366
O	-2.840110	-0.964923	1.523603
O	-1.558340	1.016543	0.205607

O	-0.268290	-1.339354	0.610737
Si	-1.719402	-0.631237	0.357790
H	-0.451185	-1.530225	-2.079919
N	0.541362	-1.331082	-2.224766
Ta	1.573603	-0.902749	0.019243
H	0.582070	-0.452303	-2.737680
H	1.564170	-3.629857	-0.907024
H	3.015947	-2.254855	-1.063786
N	2.174911	-3.002635	-0.392872
H	2.570731	-3.519688	0.385781
O	0.143376	2.745013	1.318382
O	-0.508572	3.033745	-1.247646
O	1.042779	0.925279	-0.538765
Si	-0.179647	1.915189	-0.068135
N	2.498905	-0.720458	1.526583
H	2.999363	-0.597647	2.397075
N	3.327687	-1.012849	-1.339561
H	4.213698	-0.687670	-0.966105
H	3.267112	-0.714077	-2.307838
H	0.912811	-2.054691	-2.835178
Si	-3.956209	-1.589327	-1.485180
H	-3.952575	-1.811894	-2.962585
H	-4.396732	-2.834885	-0.789102
H	-4.863413	-0.455486	-1.139405
Si	-2.869843	-0.893309	3.211666
H	-2.171999	0.334793	3.695703
H	-4.308676	-0.862240	3.605580
H	-2.214073	-2.111437	3.775207
Si	1.397121	3.723007	1.869029
H	2.519986	3.758301	0.882766
H	0.862394	5.103007	2.073811
H	1.879695	3.174176	3.171148
Si	-1.332147	2.978991	-2.709314
H	-0.919331	4.179679	-3.492622
H	-0.966854	1.739602	-3.471313
H	-2.808305	2.992610	-2.483318

E = -839.202055459
G = -839.025153

$[NH_3 \rightarrow NH]_{2q\cdot 2NH3\text{-}b}$

O	-1.765773	-1.840013	-1.220385
O	-2.311529	-1.999893	1.373016
O	-1.825615	0.408892	0.260115
O	0.228716	-1.357901	0.508859
Si	-1.370819	-1.195468	0.276563
H	0.142517	-1.531567	-2.066320
N	1.104095	-1.195301	-2.162452
Ta	1.872278	-0.298899	-0.044265
H	1.130960	-0.570202	-2.964665
H	3.643770	-2.593688	-0.236446
H	3.087349	-1.301522	1.253033
N	2.838975	-2.277099	0.291574
H	2.274633	-3.066625	0.585435
O	-0.878532	2.603795	1.473366
O	-1.430312	2.704703	-1.127606
O	0.693073	1.236199	-0.287996
Si	-0.837428	1.731102	0.076784
N	2.818644	-0.074201	1.544410
H	3.168385	0.292050	2.418381
N	3.339328	0.272355	-1.294462
H	4.229549	0.617781	-0.954987
H	3.336205	0.304635	-2.306848
H	1.684800	-2.002147	-2.378886
Si	-3.142483	-2.690657	-1.714641
H	-3.059298	-2.769227	-3.204399
H	-3.135017	-4.067991	-1.137232
H	-4.382855	-1.967059	-1.307199
Si	-2.349589	-2.080562	3.059555
H	-1.943332	-0.773680	3.657362
H	-3.753816	-2.411567	3.440865
H	-1.430327	-3.162611	3.525299
Si	-0.717034	4.237854	1.850639
H	0.418995	4.844595	1.091459
H	-1.982149	4.964992	1.528406
H	-0.448920	4.310967	3.316716
Si	-1.984165	2.454609	-2.694618
H	-1.918817	3.768152	-3.398375
H	-1.115541	1.461470	-3.404895
H	-3.389654	1.950031	-2.673738

E = -839.190865931
G = -839.016313

$[NH_2 \rightarrow NH]_{2q\cdot 2NH3\text{-}b}$

O	2.264322	-1.247798	1.337398
O	3.074018	-0.911500	-1.169141
O	1.605804	1.023286	-0.003214
O	0.417121	-1.357191	-0.590862
Si	1.800369	-0.622529	-0.148478
H	0.272517	-1.707173	2.127078
N	-0.735362	-1.552200	2.061070
Ta	-1.563716	-1.039737	-0.185252
H	-0.935023	-0.685647	2.558025
H	-1.169352	-3.885082	0.278516
H	-2.219746	-3.700555	-0.969993
N	-1.373957	-3.328115	-0.547058
H	-0.597459	-3.450422	-1.195065
O	-0.000277	2.678014	-1.313294
O	0.271388	2.946140	1.339023
O	-1.072410	0.799776	0.403576
Si	0.156566	1.839380	0.101978
N	-2.440472	-0.815207	-1.817785
H	-2.772892	-0.619305	-2.750037
N	-3.264597	-1.294838	0.581045
H	-3.343804	-1.017851	-0.800499
H	-4.122205	-1.525127	1.060029
H	-1.221677	-2.288459	2.564758
Si	3.803962	-1.377075	2.023357
H	3.586100	-1.634831	3.479418
H	4.542136	-2.526285	1.417868
H	4.579133	-0.114393	1.838190
Si	3.579235	-0.185934	-2.608322
H	4.341171	1.063214	-2.309689
H	4.472044	-1.173827	-3.284375
H	2.407168	0.125103	-3.480756
Si	-0.795690	4.094465	-1.750672
H	-2.104273	4.217170	-1.036779
H	0.059349	5.277664	-1.428802

H	-1.026141	4.025307	-3.223963
Si	-0.436088	2.969602	2.863428
H	-1.880784	3.339179	2.773969
H	-0.312766	1.631928	3.529681
H	0.301784	3.986141	3.668981

E = -839.161447739
G = -838.985267

$[NH_3 \rightarrow NH_2]_{3q \cdot NH3\text{-}a}$

O	0.994283	2.508946	-1.400244
O	1.253547	2.657927	1.239756
O	1.721365	0.316855	-0.064435
O	-0.812092	1.228386	0.193264
Si	0.769354	1.673062	0.003362
H	-0.969341	-0.580571	-2.645585
N	-1.842233	-0.381125	-2.165758
Ta	-1.847047	-0.404952	0.091555
H	-2.290456	0.395634	-2.643290
H	-3.600640	1.620272	0.282299
H	-4.527938	0.256834	0.211336
N	-3.575674	0.606276	0.214671
O	1.932254	-1.971216	1.380174
O	2.205082	-2.041337	-1.271183
O	-0.240927	-1.539432	-0.139433
Si	1.379282	-1.314561	-0.032128
N	-1.921060	-1.103811	1.961161
H	-1.278043	-1.796639	2.330136
N	-3.029401	-2.071027	-0.838365
H	-4.036621	-2.124997	-0.720007
H	-2.593996	-1.436750	-1.841767
H	-2.649614	-3.003299	-0.694367
H	-2.648787	-0.901587	2.636975
Si	1.224682	4.145029	-1.739065
H	0.149898	4.967764	-1.103230
H	2.561676	4.595889	-1.249138
H	1.153008	4.276563	-3.223786
Si	1.148985	2.619956	2.924128
H	2.173358	3.577331	3.433398
H	-0.213571	3.056302	3.355291
H	1.425895	1.243432	3.433182
Si	2.704315	-1.528475	-2.798550
H	3.146904	-2.750772	-3.530318
H	1.568362	-0.883986	-3.528008
H	3.835678	-0.562044	-2.677182
Si	3.375050	-2.745810	1.786119
H	3.402871	-2.826244	3.276121
H	3.403675	-4.120564	1.201657
H	4.549255	-1.963089	1.293476

E = -839.206859865
G = -839.033860

$[NH_3 \rightarrow NH_2]_{2q \cdot 2NH3\text{-}c}$

O	1.200473	-2.098722	1.122515
O	2.033213	-2.241036	-1.397928
O	1.792683	0.185534	-0.261158
O	-0.467388	-1.282039	-0.779382
Si	1.121272	-1.328090	-0.365259
H	-0.732416	-1.716656	1.917005
N	-1.639653	-1.240330	1.955011
Ta	-2.001106	-0.256217	-0.086301
H	-1.572710	-0.517035	2.667323
H	-3.046792	1.638243	-0.282404
H	-1.656496	2.068524	-1.562023
N	-2.411707	1.408359	-1.391442
H	-2.983867	1.297999	-2.220995
O	0.779598	2.570130	-1.067271
O	1.824193	2.343747	1.356518
O	-0.553634	1.068269	0.746459
Si	0.906980	1.532008	0.230682
N	-3.381914	-1.287328	-0.586329
H	-4.185562	-1.850249	-0.840663
N	-3.264302	1.201426	0.977960
H	-4.231249	1.023849	1.224200
H	-2.838739	1.831608	1.650522
H	-2.349618	-1.911248	2.234285
Si	2.366860	-3.169335	1.724572
H	2.063998	-3.316380	3.180368
H	2.251685	-4.494791	1.047616
H	3.739104	-2.610653	1.541545
Si	2.678858	-1.984581	-2.937442
H	1.781560	-1.099809	-3.740183
H	4.030806	-1.361725	-2.813929
H	2.793682	-3.324910	-3.583062
Si	1.809522	3.772226	-1.647395
H	1.734797	4.986815	-0.779729
H	3.220391	3.281960	-1.708076
H	1.330141	4.108425	-3.021819
Si	2.571254	1.914780	2.799022
H	2.867190	3.180633	3.532240
H	1.666877	1.054136	3.626218
H	3.841452	1.175038	2.528577

E = -839.199608482
G = -839.020503

$[NH_3 \rightarrow NH]_{2q \cdot 2NH3\text{-}c}$

O	-1.046004	-2.185020	-1.236809
O	-1.767227	-2.495815	1.298847
O	-1.811514	-0.028980	0.213320
O	0.597367	-1.226850	0.637621
Si	-0.970741	-1.464673	0.278669
H	0.724369	-1.403407	-2.037536
N	1.524488	-0.765565	-2.096098
Ta	2.022784	0.073258	0.007938
H	1.283994	-0.024391	-2.750705
H	3.017401	1.076908	2.458541
H	2.015964	-0.212828	2.787440
N	2.613852	0.221955	2.092603
H	3.390309	-0.582536	1.325510
O	-1.363957	2.404408	1.301640
O	-1.959992	2.219467	-1.275713
O	0.465775	1.320695	-0.378934
Si	-1.123662	1.473176	-0.044624
N	3.545302	-1.027793	0.072365
H	4.346712	-1.629023	-0.063460

N	3.028037	1.666294	-0.663770
H	4.027753	1.733293	-0.814768
H	2.570136	2.544991	-0.884677
H	2.314924	-1.280046	-2.475162
Si	-2.095463	-3.377991	-1.819948
H	-1.832425	-3.464387	-3.288457
H	-1.799921	-4.691847	-1.175648
H	-3.517946	-2.992925	-1.579238
Si	-2.351237	-2.390137	2.878139
H	-2.552935	-3.790635	3.351817
H	-1.361956	-1.690159	3.753652
H	-3.649931	-1.652740	2.892803
Si	-2.420022	3.669988	1.644945
H	-2.072395	4.877743	0.835392
H	-3.834769	3.272584	1.369532
H	-2.253776	3.972474	3.097579
Si	-2.497353	1.735559	-2.791455
H	-2.800666	2.973923	-3.566563
H	-1.432692	0.953050	-3.499726
H	-3.724047	0.891738	-2.671452

E = -839.187514652
G = -839.009664

$[NH_3 \rightarrow NH_2]_{2q \cdot 2NH3\text{-}d}$

O	1.200473	-2.098722	1.122515
O	2.033213	-2.241036	-1.397928
O	1.792683	0.185534	-0.261158
O	-0.467388	-1.282039	-0.779382
Si	1.121272	-1.328090	-0.365259
H	-0.732416	-1.716656	1.917005
N	-1.639653	-1.240330	1.955011
Ta	-2.001106	-0.256217	-0.086301
H	-1.572710	-0.517035	2.667323
H	-3.046792	1.638243	-0.282404
H	-1.656496	2.068524	-1.562023
N	-2.411707	1.408359	-1.391442
H	-2.983867	1.297999	-2.220995
O	0.779598	2.570130	-1.067271
O	1.824193	2.343747	1.356518
O	-0.553634	1.068269	0.746459
Si	0.906980	1.532008	0.230682
N	-3.381914	-1.287328	-0.586329
H	-4.185562	-1.850249	-0.840663
N	-3.264302	1.201426	0.977960
H	-4.231249	1.023849	1.224200
H	-2.838739	1.831608	1.650522
H	-2.349618	-1.911248	2.234285
Si	2.366860	-3.169335	1.724572
H	2.063998	-3.316380	3.180368
H	2.251685	-4.494791	1.047616
H	3.739104	-2.610653	1.541545
Si	2.678858	-1.984581	-2.937442
H	1.781560	-1.099809	-3.740183
H	4.030806	-1.361725	-2.813929
H	2.793682	-3.324910	-3.583062
Si	1.809522	3.772226	-1.647395
H	1.734797	4.986815	-0.779729
H	3.220391	3.281960	-1.708076
H	1.330141	4.108425	-3.021819
Si	2.571254	1.914780	2.799022
H	2.867190	3.180633	3.532240
H	1.666877	1.054136	3.626218
H	3.841452	1.175038	2.528577

E = -839.199608482
G = -839.020503

$[NH_3 \rightarrow NH]_{2q \cdot 2NH3\text{-}d}$

O	-0.400833	2.720850	1.199293
O	-0.959328	2.875321	-1.405385
O	-1.712031	0.710764	0.024043
O	0.909400	1.096405	-0.569477
Si	-0.509594	1.840899	-0.191245
H	1.709658	-0.383112	2.620480
N	2.355460	-0.293836	1.842759
Ta	1.801674	-0.571197	-0.034297
H	3.282937	-0.048130	2.166203
H	4.300534	-0.083062	-1.376843
H	3.443238	-1.674055	-0.638577
N	3.492354	-0.385312	-0.848721
O	-1.987464	-1.751335	-1.043395
O	-2.614099	-1.364459	1.504055
O	0.022272	-1.263503	0.674679
Si	-1.530121	-0.919234	0.336131
N	2.625377	-2.649962	-0.180064
H	2.823158	-3.104297	0.705975
N	0.867333	-1.290326	-2.121544
H	0.756133	-0.460578	-2.701257
H	1.447176	-1.940071	-2.645595
H	-0.060877	-1.704418	-2.006908
H	2.233774	-3.344055	-0.807644
Si	0.387137	4.132056	1.671617
H	1.679635	4.290906	0.937767
H	-0.492709	5.309490	1.402518
H	0.642031	4.017165	3.137941
Si	-1.626936	2.662961	-2.932762
H	-1.308999	3.884462	-3.727498
H	-1.028916	1.461566	-3.601513
H	-3.105665	2.480762	-2.832936
Si	-2.994227	-0.815420	3.053895
H	-3.746910	-1.917842	3.720708
H	-1.746922	-0.510714	3.819378
H	-3.846156	0.407759	2.966271
Si	-3.465184	-2.469504	-1.447293
H	-3.352481	-2.843619	-2.889546
H	-3.690448	-3.694579	-0.624023
H	-4.590509	-1.506400	-1.257497

E = -839.192295632
G = -839.016163

$[2q \cdot NH_3]NH_{3a}$

O	-0.928365	2.881554	1.131203
O	-1.194018	2.464610	-1.479888
O	-1.816570	0.486666	0.273909
O	0.773083	1.183351	-0.160728
Si	-0.766643	1.734759	-0.059339

H	2.429422	-2.096565	1.527937
N	2.806092	-1.750736	0.649601
Ta	1.707567	-0.547429	-0.545561
H	3.482228	-2.419769	0.298223
H	3.048555	1.913240	-0.592358
H	3.826959	1.058171	0.603187
N	3.420569	0.998574	-0.345840
H	4.177767	0.787997	-0.990972
O	-2.682667	-1.921403	-0.612831
O	-1.716319	-1.677778	1.850307
O	-0.010758	-1.454304	-0.249145
Si	-1.528808	-1.150614	0.291534
N	2.183367	-0.923030	-2.218162
H	2.218274	-1.019552	-3.224512
Si	-1.115737	2.806986	2.802653
H	-0.148252	1.830680	3.396290
H	-0.829137	4.175369	3.326352
H	-2.509965	2.406491	3.156646
Si	-2.778674	-2.787245	2.544519
H	-2.615517	-4.135714	1.920493
H	-2.417274	-2.855801	3.992011
H	-4.193269	-2.329871	2.396748
Si	-2.836582	-2.281469	-2.254308
H	-2.028895	-3.493312	-2.587346
H	-4.283844	-2.555594	-2.494288
H	-2.387732	-1.127115	-3.090557
Si	-2.270423	3.704962	-1.854531
H	-1.676149	5.028149	-1.492755
H	-2.497873	3.640418	-3.328346
H	-3.565225	3.522557	-1.129612
H	4.181342	-0.356647	2.222030
N	4.504102	0.595012	2.403585
H	5.488050	0.538604	2.653920
H	4.010298	0.926977	3.228567

E = -839.221183247
G = -839.048851

$[2q{\cdot}NH_3]NH_{3b}$

O	1.586034	2.734873	-1.137049
O	0.977302	2.532293	1.444466
O	1.963240	0.378253	0.116664
O	-0.566487	1.254758	-0.349233
Si	0.967583	1.707624	0.011045
H	-2.219875	-1.785331	-2.396103
N	-2.600530	-1.565879	-1.480968
Ta	-1.723393	-0.363985	-0.144389
H	-3.417579	-2.139712	-1.309814
H	-3.146430	1.355918	-1.945801
H	-4.125944	1.099169	-0.629505
N	-3.152202	1.276263	-0.931889
H	-2.857191	2.177771	-0.562346
O	2.274117	-2.012100	1.358969
O	2.212774	-1.867427	-1.297902
O	-0.073570	-1.399239	0.109145
Si	1.558375	-1.233390	0.083195
N	-2.650307	-0.560758	1.374202
H	-2.796706	-0.576217	2.376283
Si	2.320580	2.489275	-2.633740
H	1.541642	1.500650	-3.443197
H	2.324929	3.812261	-3.325598
H	3.720531	2.002107	-2.455208
Si	3.054288	-3.293536	-1.609121
H	2.302353	-4.477402	-1.089964
H	3.179867	-3.388811	-3.094000
H	4.411863	-3.247857	-0.987229
Si	1.787356	-2.315255	2.945384
H	0.871787	-3.495473	2.981851
H	3.026707	-2.612788	3.721720
H	1.096205	-1.122110	3.522532
Si	2.002125	3.704032	2.088290
H	1.695516	5.038837	1.489094
H	1.739048	3.738946	3.557370
H	3.433985	3.357412	1.834117
H	-4.920710	-0.128389	0.932521
N	-5.635595	0.411508	0.437911
H	-6.107882	0.988803	1.129166
H	-6.325593	-0.248594	0.088474

E = -839.223184104
G = -839.049005

$[NH_3\text{-}NH_2]_{[2q\cdot NH3]NH3a}$

O	-1.325226	2.562475	1.564622
O	-1.513017	2.541997	-1.088439
O	-1.925186	0.270118	0.251637
O	0.584899	1.278737	0.125475
Si	-1.009492	1.655500	0.210137
H	2.109271	-2.768019	0.324673
N	2.778744	-2.009971	0.196745
Ta	1.741741	-0.222079	-0.464686
H	3.430877	-2.347627	-0.510549
H	2.873611	1.653382	1.097711
H	3.848837	-0.120886	1.722075
N	3.265557	0.806038	0.688611
H	4.031369	1.125958	0.096536
O	-2.445527	-1.970572	-1.170017
O	-1.730568	-2.168158	1.376712
O	0.123872	-1.371728	-0.411420
Si	-1.463448	-1.306479	-0.013323
N	2.299850	-0.015329	-2.136682
H	2.375996	0.160443	-3.129352
Si	-1.438460	2.221228	3.206590
H	-0.309118	1.337249	3.639515
H	-1.353863	3.525920	3.926978
H	-2.737142	1.550783	3.513851
Si	-3.024086	-3.116650	1.892292
H	-3.042378	-4.417597	1.156204
H	-2.802751	-3.369259	3.347881
H	-4.322957	-2.405361	1.692275
Si	-2.571861	-1.822978	-2.845139
H	-1.656010	-2.803591	-3.503655
H	-3.986598	-2.139567	-3.200503
H	-2.227860	-0.436321	-3.281197
Si	-1.419986	4.163600	-1.524866
H	-0.085579	4.735815	-1.164174
H	-1.614515	4.224994	-3.003511
H	-2.496867	4.941989	-0.840346

H	3.571683	-1.719875	1.441382
N	4.119485	-1.107800	2.248086
H	5.117535	-1.288981	2.296392
H	3.712608	-1.200266	3.174354

E = -839.193789504
G = -839.022071

$[NH_3\text{-}NH]_{[2q\cdot NH3]NH3b}$

O	1.182112	2.656673	-1.353133
O	0.587985	2.648131	1.227364
O	1.796645	0.488904	0.138003
O	-0.803800	1.017599	-0.421895
Si	0.650536	1.677972	-0.116977
H	-2.236934	-3.010866	-1.531816
N	-2.572935	-2.460833	-0.747794
Ta	-1.801463	-0.722268	-0.098676
H	-3.347140	-2.943214	-0.306794
H	-3.656182	-0.240497	-2.069709
H	-4.090109	1.061425	-0.315047
N	-3.119014	0.321651	-1.415380
H	-2.673908	1.074262	-1.936476
O	2.360647	-1.799682	1.460118
O	2.275358	-1.815959	-1.195911
O	-0.028941	-1.519153	0.166366
Si	1.572052	-1.158628	0.149897
N	-2.732769	-0.480342	1.477530
H	-2.568264	-0.704663	2.455385
Si	1.894794	2.362623	-2.849313
H	1.210397	1.230103	-3.547215
H	1.741386	3.613819	-3.650173
H	3.344952	2.045276	-2.681666
Si	3.692926	-2.696973	-1.425480
H	3.593549	-4.033285	-0.763881
H	3.840150	-2.873459	-2.900838
H	4.873257	-1.955221	-0.885281
Si	2.512328	-1.331941	3.072069
H	2.878135	-2.556668	3.842943
H	3.591179	-0.307348	3.207472
H	1.222304	-0.774308	3.582687
Si	1.382245	4.077745	1.622283
H	0.796853	5.227114	0.864857
H	1.170169	4.288969	3.085969
H	2.845575	3.981743	1.332186
H	-3.832086	0.612437	1.234235
N	-4.476029	1.343227	0.681989
H	-4.248464	2.304601	0.917725
H	-5.471147	1.176142	0.792339

E = -839.196504790
G = -839.022443

$[2q\cdot 2NH_3]NH_{3a}$

O	-1.492122	-2.250078	-1.076558
O	-2.252339	-2.206222	1.456120
O	-2.119939	0.110574	0.081611
O	0.199081	-1.180671	0.710053
Si	-1.370464	-1.353827	0.341085
H	0.349647	-1.613435	-1.926808
N	1.160388	-1.001759	-2.050863
Ta	1.663575	0.139233	0.124721
H	0.862529	-0.262382	-2.684616
H	2.251762	-2.639725	0.174091
H	3.754945	-1.904791	0.154170
N	2.788754	-1.846056	0.514490
H	2.824781	-1.944656	1.526443
O	-1.588758	2.484009	1.183683
O	-2.129693	2.356487	-1.414101
O	0.220685	1.329972	-0.542914
Si	-1.355876	1.571418	-0.172038
N	2.232591	0.881428	1.642683
H	2.505540	1.310488	2.517042
N	3.181949	0.795856	-1.078403
H	3.796167	1.538541	-0.762801
H	3.187059	0.778364	-2.092599
H	1.881809	-1.534407	-2.530322
Si	-2.719149	-3.285044	-1.604290
H	-2.479442	-3.496172	-3.064843
H	-2.632485	-4.596148	-0.892774
H	-4.064360	-2.673222	-1.392102
Si	-2.569984	-2.027575	3.102348
H	-2.782042	-0.591110	3.450792
H	-3.804852	-2.816951	3.386523
H	-1.429282	-2.578994	3.896749
Si	-1.009216	3.962118	1.735890
H	-0.079100	4.583115	0.743822
H	-2.178317	4.865429	1.961919
H	-0.295763	3.741621	3.029915
Si	-2.603731	1.913457	-2.959797
H	-2.741195	3.165782	-3.760345
H	-1.575779	1.028248	-3.599586
H	-3.909636	1.188263	-2.920627
N	5.498316	-1.436505	-0.644051
H	4.994077	-0.582662	-0.904427
H	6.243165	-1.163386	-0.007678
H	5.948375	-1.796784	-1.481478

E = -895.792187968
G = -895.578848

$[2q\cdot 2NH_3]NH_{3b}$

O	-1.972844	-1.619026	-1.341155
O	-2.303335	-2.004386	1.272616
O	-1.865759	0.488648	0.369432
O	0.163091	-1.344214	0.247786
Si	-1.438429	-1.110239	0.169420
H	-0.190591	-1.137644	-2.406878
N	0.717728	-0.695120	-2.566119
Ta	1.782625	-0.218521	-0.355872
H	0.522896	0.231047	-2.942214
H	3.485660	-2.469142	-0.779468
H	2.406581	-2.818563	0.446121
N	2.510769	-2.402051	-0.500409
H	1.961658	-2.973377	-1.137437
O	-0.559726	2.334165	1.780643
O	-1.594852	3.005660	-0.569752
O	0.539302	1.330647	-0.544995

Si	-0.819445	1.785811	0.244332
N	2.689162	0.099874	1.152571
H	3.201183	0.359016	1.985705
N	3.232558	0.317324	-1.658288
H	4.126278	0.687066	-1.356987
H	3.196408	0.323222	-2.670858
H	1.196379	-1.220747	-3.293058
Si	-3.455374	-2.296754	-1.786307
H	-3.516156	-2.214753	-3.277457
H	-3.518267	-3.728244	-1.362513
H	-4.592038	-1.535790	-1.187138
Si	-2.938076	-1.603915	2.785628
H	-4.085688	-0.660400	2.639875
H	-3.409271	-2.887408	3.387249
H	-1.882954	-0.997404	3.653192
Si	0.493993	3.442181	2.479397
H	1.361959	4.089892	1.449291
H	-0.322008	4.482733	3.176144
H	1.342179	2.728287	3.481225
Si	-2.279087	3.158021	-2.093165
H	-2.070793	4.565012	-2.546672
H	-1.631269	2.220844	-3.067345
H	-3.741815	2.858152	-2.028845
N	1.932914	-3.033744	2.295682
H	2.005952	-2.022047	2.411951
H	0.938432	-3.244996	2.328279
H	2.364558	-3.470135	3.105558

E = -895.794513361
G = -895.579819

$[NH_3\text{-}NH_2]_{[2q\cdot 2NH3]NH3a}$

O	-1.909886	-1.921255	-1.124800
O	-2.667809	-1.765711	1.408748
O	-2.078182	0.497439	0.059278
O	-0.062390	-1.213244	0.697898
Si	-1.634517	-1.086612	0.305625
H	0.064725	-1.615425	-1.974162
N	0.921424	-1.070468	-2.097873
Ta	1.634263	-0.257699	0.171351
H	0.651118	-0.241590	-2.623947
H	2.145305	-2.910065	-0.420800
H	4.022487	-1.953793	-0.388886
N	2.638274	-2.189831	0.104431
H	2.724228	-2.561754	1.049534
O	-1.152994	2.729899	1.200911
O	-1.624748	2.707049	-1.408854
O	0.473282	1.262648	-0.472241
Si	-1.039264	1.787405	-0.152211
N	2.341900	0.269457	1.720599
H	2.684176	0.586931	2.617745
N	3.236897	0.529832	-1.073763
H	3.593224	1.393466	-0.666515
H	2.973696	0.773231	-2.027048
H	1.549587	-1.612292	-2.685581
Si	-3.247667	-2.827256	-1.617398
H	-3.046028	-3.094373	-3.074681
H	-3.301166	-4.124705	-0.878232
H	-4.515427	-2.066165	-1.411045
Si	-2.775307	-1.711645	3.091308
H	-2.410919	-0.356794	3.602886
H	-4.191450	-2.031399	3.439438
H	-1.868596	-2.740475	3.686395
Si	-0.210327	3.936549	1.890570
H	0.814261	4.442263	0.925216
H	-1.121173	5.054005	2.283804
H	0.470357	3.399941	3.107774
Si	-2.192215	2.336302	-2.940176
H	-2.141460	3.589511	-3.749954
H	-1.324599	1.298502	-3.591498
H	-3.594176	1.823079	-2.882248
N	4.960122	-1.414254	-0.806486
H	4.350424	-0.452573	-1.032829
H	5.673027	-1.266907	-0.098101
H	5.378851	-1.854765	-1.619814

E = -895.764301785
G = -895.554077

$[NH_3\text{-}NH_2]_{[2q\cdot 2NH3]NH3b}$

O	1.212318	2.246734	-1.280277
O	1.412315	2.749062	1.314085
O	1.886282	0.255075	0.431811
O	-0.667555	1.223750	0.339061
Si	0.904745	1.590490	0.236673
H	-0.298256	1.154250	-2.329680
N	-1.006834	0.438150	-2.504380
Ta	-1.805078	-0.376769	-0.291407
H	-0.542697	-0.323608	-2.993946
H	-3.961608	1.188926	-1.066077
H	-3.874050	1.169382	1.071015
N	-3.228522	1.251033	-0.363817
H	-2.797698	2.169801	-0.442371
O	1.461409	-2.123875	1.617057
O	2.545192	-2.069523	-0.792001
O	-0.073006	-1.354445	-0.512495
Si	1.409668	-1.322386	0.168619
N	-2.441993	-1.108918	1.287638
H	-2.262562	-1.877968	1.926097
N	-2.923793	-1.482761	-1.556174
H	-3.562218	-2.200919	-1.235521
H	-2.934689	-1.457928	-2.569063
H	-1.696598	0.840117	-3.133521
Si	2.318349	3.437858	-1.737490
H	2.362233	3.408566	-3.231495
H	1.856506	4.783011	-1.279325
H	3.675591	3.148931	-1.184815
Si	1.838062	2.706703	2.943422
H	3.225294	2.176570	3.104178
H	1.776632	4.115832	3.435311
H	0.880984	1.859490	3.719896
Si	2.338682	-3.456386	2.148969
H	2.036726	-4.661991	1.317274
H	3.807196	-3.178364	2.110894
H	1.912063	-3.702806	3.559278
Si	3.178042	-1.825104	-2.326346
H	3.826843	-3.102042	-2.745657
H	2.093688	-1.474353	-3.299478

H	4.188025	-0.723536	-2.305937
N	-4.081352	0.777999	2.105684
H	-3.424476	-0.130948	1.941870
H	-3.723307	1.388181	2.833597
H	-5.056771	0.556332	2.275752

E = -895.766059404
G = -895.555444