Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplement 1: Cartesian coordinates of all stationary points along reaction pathways

1 $SiH_4 \longrightarrow SiH_3^{\cdot} + H^{\cdot}$

This reaction does not have the transition state. Only two geometries are used in calculating reaction energetics: the reactant and products.

1.1 SiH_4 (reactant)

All coordinates are in Ångström units.

Si	-0.0000582558	0.0000000000	-0.0408343922
H	0.0001053706	0.0000000000	1.4343035664
H	-0.6953489450	-1.2043591271	-0.5326361355
H	-0.6953489450	1.2043591271	-0.5326361355
H	1.3906507759	0.0000000000	-0.5325076485

1.2 $SiH_3^{\cdot} + H^{\cdot}$ (products)

This geometry is created by placing one of the hydrogen atoms 20Å from the silicon atom and optimising by implying the triplet state. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.0000135596	0.0000000000	-0.0805055669
H	-0.0000000088	0.0000000000	19.9998344715
H	-0.7023964687	-1.2166252912	-0.5312117018
H	-0.7023964687	1.2166252912	-0.5312117018
H	1.4048065056	0.0000000000	-0.5312162463

2 $SiH_4 \longrightarrow SiH_2 + H_2$

2.1 SiH_4 (reactant)

All coordinates are in Ångström units.

Si	0.0000000000	-0.0000000000	0.0000000000
H	0.0000000000	-1.2044982383	0.8514811493
H	-1.2044982383	0.0000000000	-0.8514811493
H	1.2044982383	0.0000000000	-0.8514811493
H	0.0000000000	1.2044982383	0.8514811493

2.2 $SiH_2 + H_2$ (products)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.000000	-0.127600
H	0.000000	-0.500000	21.872400
H	-1.204435	-0.000000	-0.979204
H	1.204435	0.000000	-0.979204
H	0.000000	0.500000	21.872400

3 $NH_3 \longrightarrow \dot{N}H_2 + H^{\cdot}$

3.1 NH_3 (reactant)

All coordinates are in Ångström units.

N	-0.0000000000	0.0000000000	-0.2907664378
H	-0.4690310598	0.8123856258	-0.6708090937
H	-0.4690310598	-0.8123856258	-0.6708090937
H	0.9380621195	0.0000000000	-0.6708090937

3.2 $\dot{N}H_2 + H^{\cdot}$ (products)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	-0.000000	-0.000000	0.410039
H	-0.469031	0.812386	0.029987
H	-0.469031	-0.812386	0.029987
H	92.691585	0.000000	-37.143526

4 $NH_3 + SiH_4 \longrightarrow H_2N{-}SiH_3 + H_2$

4.1 $NH_3 + SiH_4$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.372073	0.013879	0.000000
H	2.209622	-0.158764	-1.202957
H	2.209622	-0.158764	1.202957
H	0.768730	1.356938	0.000000
H	0.313377	-1.014728	0.000000
H	-23.558023	0.216490	0.000000
H	-22.288499	-0.393693	-0.811189
H	-22.288499	-0.393693	0.811189
N	-22.547518	0.153787	0.000000

4.2 $NH_3 + SiH_4$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	14.0	1.3720726670	0.0138790973	0.0000000000
H	1.0	2.2096223009	-0.1587643753	-1.2029570035
H	1.0	2.2096223009	-0.1587643753	1.2029570035
H	1.0	0.7687304451	1.3569379399	0.0000000000
H	1.0	0.3133766121	-1.0147281189	0.0000000000
H	1.0	-3.5614913762	0.0995284969	0.0000000000
H	1.0	-2.2919675605	-0.5106543892	-0.8111891638
H	1.0	-2.2919675605	-0.5106543892	0.8111891638
N	7.0	-2.5509869812	0.0368254818	0.0000000000

4.3 transition state

All coordinates are in Ångström units.

Si	0.6500220788	-0.0283072114	0.0000000000
H	1.3001679030	0.3200892396	-1.2748237344
H	1.3001679030	0.3200892396	1.2748237344
H	0.0520990384	1.7277708120	0.0000000000
H	0.7642782109	-1.5309460688	0.0000000000
H	-0.9372313641	1.1268326950	0.0000000000
H	-1.6830812976	-0.4014322490	-0.8301496736
H	-1.6830812976	-0.4014322490	0.8301496736
N	-1.2348748365	-0.0270145450	0.0000000000

4.4 $NH_2-SiH_3 + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.6026664659	-0.1543027853	0.0000000000
H	1.0826123256	0.5323979136	-1.2147935048
H	1.0826123256	0.5323979136	1.2147935048
H	-0.4422982347	3.5303275793	0.0000000000
H	1.1765276468	-1.5215687622	0.0000000000
H	-0.7328087475	2.8506494678	0.0000000000
H	-1.6327058935	-0.3451844120	-0.8256836281
H	-1.6327058935	-0.3451844120	0.8256836281
N	-1.1249983884	-0.0684189943	0.0000000000

4.5 $NH_2-SiH_3 + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecu-

lar fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.602666	-0.154303	0.000000
H	1.082612	0.532398	-1.214794
H	1.082612	0.532398	1.214794
H	2.221487	23.356885	0.000000
H	1.176528	-1.521569	0.000000
H	1.930976	22.677207	0.000000
H	-1.632706	-0.345184	-0.825684
H	-1.632706	-0.345184	0.825684
N	-1.124998	-0.068419	0.000000

5 $NH_2{-}SiH_3 + NH_3 \longrightarrow NH_2{-}SiH_2{-}NH_2 + H_2$

5.1 $NH_2{-}SiH_3 + NH_3$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of the reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.449097	-0.257214	0.089404
H	0.797326	0.348369	-1.208228
H	0.941240	0.512954	1.245410
H	0.992408	-1.634296	0.149684
H	-1.839650	-0.524277	-0.585979
H	-1.743432	-0.413490	1.056018
N	-1.287532	-0.184863	0.186373
N	23.387384	0.866588	-1.336145
H	23.744797	1.811375	-1.408682
H	23.825569	0.448573	-0.524464
H	23.727420	0.361227	-2.145341

5.2 $NH_2-SiH_3 + NH_3$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.4490973736	-0.2572138497	0.0894039690
H	0.7973259033	0.3483689860	-1.2082282425
H	0.9412400011	0.5129537027	1.2454096632
H	0.9924083284	-1.6342961176	0.1496842050
H	-1.8396502762	-0.5242768764	-0.5859788650
H	-1.7434319920	-0.4134897375	1.0560183148
N	-1.2875321330	-0.1848628142	0.1863733016
N	3.4509110736	-0.1101478329	-0.0971502138
H	3.8083239697	0.8346392130	-0.1696873543
H	3.8890968519	-0.5281619136	0.7145309516
H	3.7909477909	-0.6155087580	-0.9063462657

5.3 transition state

All coordinates are in Ångström units.

Si	0.7476299845	-0.6688696153	0.2059113036
H	0.9408134624	-0.4008983962	-1.6110749844
H	0.7615570157	-0.7002282606	1.7075644433
H	0.9377931330	-2.0944555695	-0.1284767799
H	-1.0457756892	0.5213934925	-0.8769490593
H	-1.2524280361	0.4923432909	0.7993292357
N	-0.6402018254	0.3145701951	0.0194849469
N	2.4017236910	0.1655518018	-0.0783992635
H	2.4308480333	1.1456771433	0.1788407287
H	3.2457037570	-0.3085568604	0.2225151184
H	1.9141104740	-0.0175412217	-1.1722786895

5.4 $NH_2-SiH_2-NH_2 + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.8026616693	-0.6718256071	0.3964564998
H	0.7806308989	0.1229708365	-3.4038587600
H	0.5784614067	-0.8964673209	1.8439448295
H	0.9320918967	-1.9934257217	-0.2608811474
H	-0.6714173822	0.5777624530	-1.0320174155
H	-1.3889441703	0.2806939698	0.4425629977
N	-0.5241969151	0.3130593614	-0.0716180395
N	2.2453437392	0.1466109799	-0.0601266661
H	2.4476125535	1.0718933328	0.2834168757
H	3.0900976510	-0.3744856702	-0.2314329088
H	1.1974094502	0.2150335134	-2.7998082482

5.5 $NH_2-SiH_2-NH_2 + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.802662	-0.671826	0.396456
H	3.144037	5.432712	-22.540313
H	0.578461	-0.896467	1.843945
H	0.932092	-1.993426	-0.260881
H	-0.671417	0.577762	-1.032017
H	-1.388944	0.280694	0.442563
N	-0.524197	0.313059	-0.071618
N	2.245344	0.146611	-0.060127
H	2.447613	1.071893	0.283417
H	3.090098	-0.374486	-0.231433
H	3.560816	5.524775	-21.936262

6 $(NH_2)_2SiH_2 + NH_3 \longrightarrow (NH_2)_3SiH + H_2$

6.1 $(NH_2)_2SiH_2 + NH_3$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.936748	0.146562	0.873312
H	0.323999	1.208422	0.032214
H	0.705803	0.519290	2.290969
H	-18.315312	-2.260359	-12.444392
H	-18.795890	-3.486023	-13.399191
H	-19.662784	-3.095828	-12.079838
N	-18.718909	-3.189983	-12.433960
N	2.647750	-0.014640	0.786999
H	3.111044	-0.242774	-0.077412
H	3.245213	0.513619	1.401338
N	0.215536	-1.289031	0.292625
H	0.406041	-2.187056	0.705276
H	-0.682108	-1.248857	-0.177174

6.2 $(NH_2)_2SiH_2 + NH_3$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.6187983503	-0.0973572190	-0.2228909105
H	0.6264987939	1.4251529457	-0.3274862797
H	0.2541327520	-1.5787152659	-0.1862303063
H	-1.7332526714	1.0291102758	-0.2412200092
H	-1.5068993534	0.1102851152	-1.5873146085
H	-1.9371379529	-0.6171064910	-0.1752571202
N	-1.3897953711	0.1359519076	-0.5782028494
N	1.4938904602	-0.2757573017	-1.7137024753
N	1.0193871090	-0.0676478358	1.4635449120
H	1.8093366420	-1.1765919985	-2.0378668685
H	1.1838281663	-0.9106773795	1.9903551412
H	2.0159757911	0.4870562596	-2.1156446348
H	1.3903736655	0.7548558901	1.9118928372

6.3 transition state

All coordinates are in Ångström units.

Si	0.6221780776	-0.0409905678	-0.0888831524
H	1.0432319373	0.4013634513	-1.4345446702
H	0.1721122675	1.7330277217	0.1416246010
H	-0.8282623654	1.2064590670	0.0149991302
H	-1.7471946054	-0.1891492698	-0.9512799761
H	-1.7185629476	-0.2766336112	0.7126985286
N	-1.2527377927	0.0859585235	-0.1110685983
N	1.4996673325	0.1990853622	1.3560644832
H	1.8849547333	-0.5692559267	1.8793095283
H	1.6902417884	1.1055639755	1.7422768219
N	0.7154855563	-1.8098899202	-0.0941828796
H	1.6450703377	-2.2090951954	-0.0830219741
H	0.1860046805	-2.2980486099	-0.8034568424

6.4 $(NH_2)_3SiH + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.5492817264	-0.1905402284	-0.0730491390
H	1.0483508974	0.6697161834	-1.1690714006
H	-0.1037792277	3.6851528889	0.3890231148
H	-0.2460857323	3.0656652713	0.7648502447
H	-1.5648269913	0.8760341637	-0.4338031323
H	-1.7713187766	-0.4976216354	0.4807320596
N	-1.1605402627	-0.0009231075	-0.1481448154
N	1.4900327057	0.2892523747	1.2870357668
H	1.3770666027	-0.1535679645	2.1850048173
H	1.7939470193	1.2442209770	1.3862581186
N	0.7707862390	-1.8916750294	-0.1375629102
H	1.6808516046	-2.2915557503	0.0215510188
H	0.2214269981	-2.4516646790	-0.7684711001

6.5 $(NH_2)_3SiH + H_2$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.549282	-0.190540	-0.073049
H	1.048351	0.669716	-1.169071
H	-4.708963	22.538607	5.240467
H	-4.851269	21.919119	5.616294
H	-1.564827	0.876034	-0.433803
H	-1.771319	-0.497622	0.480732
N	-1.160540	-0.000923	-0.148145
N	1.490033	0.289252	1.287036
H	1.377067	-0.153568	2.185005
H	1.793947	1.244221	1.386258
N	0.770786	-1.891675	-0.137563
H	1.680852	-2.291556	0.021551
H	0.221427	-2.451665	-0.768471

7 $(NH_2)_3SiH + NH_3 \longrightarrow (NH_2)_4Si + H_2$

7.1 $(NH_2)_3SiH + NH_3$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.670730	0.000000	0.209430
N	-0.334046	-1.516669	-0.540328
N	-0.334046	1.516669	-0.540328
N	-2.380231	0.000000	0.397332
H	0.169127	0.000000	1.430205
H	0.638134	-1.757355	-0.668644
H	0.638134	1.757355	-0.668644
H	-2.845934	-0.831172	0.723979
H	-2.845934	0.831172	0.723979
H	-0.864402	-1.777525	-1.358599
H	-0.864402	1.777525	-1.358599
H	22.400230	0.000000	0.913446
N	22.898595	0.000000	0.031032
H	23.506614	-0.810289	0.039726
H	23.506614	0.810289	0.039726

7.2 $(NH_2)_3SiH + NH_3$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.67072983	0.00000000	0.20943017
N	-0.33404571	-1.51666851	-0.54032775
N	-0.33404571	1.51666851	-0.54032775
N	-2.38023115	0.00000000	0.39733194
H	0.16912654	0.00000000	1.43020527
H	0.63813443	-1.75735503	-0.66864405
H	0.63813443	1.75735503	-0.66864405
H	-2.84593396	-0.83117189	0.72397862
H	-2.84593396	0.83117189	0.72397862
H	-0.86440187	-1.77752480	-1.35859923
H	-0.86440187	1.77752480	-1.35859923
H	2.40017404	0.00000000	1.06482799
N	2.89853881	0.00000000	0.18241408
H	3.50655797	-0.81028853	0.19110832
H	3.50655797	0.81028853	0.19110832

7.3 transition state

All coordinates are in Ångström units.

Si	-0.0944498060	0.0000000000	0.0965176792
N	-0.0155417294	-1.5834775940	-0.5682637355
N	-0.0155417294	1.5834775940	-0.5682637355
N	-1.8385377395	0.0000000000	0.3596969073
H	0.1200554955	0.0000000000	1.8503086251
H	0.8165270229	-1.9682959138	-0.9801031463
H	0.8165270229	1.9682959138	-0.9801031463
H	-2.2165072379	-0.8158937654	0.8220235164
H	-2.2165072379	0.8158937654	0.8220235164
H	-0.8513420152	-2.0129800078	-0.9307093266
H	-0.8513420152	2.0129800078	-0.9307093266
H	1.0387272088	0.0000000000	1.5245958395
N	1.8155903574	0.0000000000	0.4177995419
H	2.3670997015	-0.8306486256	0.2465693955
H	2.3670997015	0.8306486256	0.2465693955

7.4 $(NH_2)_4Si + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.02324810	0.00000000	-0.09230713
N	-0.05212997	-1.52718453	-0.88828797
N	-0.05212997	1.52718453	-0.88828797
N	-1.51804882	0.00000000	0.76307510
H	0.13311897	0.00000000	4.20845671
H	0.76010193	-1.84308815	-1.39343830
H	0.76010193	1.84308815	-1.39343830
H	-1.82381550	-0.83050496	1.24388998
H	-1.82381550	0.83050496	1.24388998
H	-0.89885260	-1.84300401	-1.33327297
H	-0.89885260	1.84300401	-1.33327297
H	0.10617807	0.00000000	3.46984788
N	1.52956473	0.00000000	0.65261143
H	1.86927526	-0.83050187	1.11007540
H	1.86927526	0.83050187	1.11007540

7.5 $(NH_2)_4Si + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.023248	0.000000	-0.092307
N	-0.052130	-1.527185	-0.888288
N	-0.052130	1.527185	-0.888288
N	-1.518049	0.000000	0.763075
H	0.859150	0.000000	24.190766
H	0.760102	-1.843088	-1.393438
H	0.760102	1.843088	-1.393438
H	-1.823816	-0.830505	1.243890
H	-1.823816	0.830505	1.243890
H	-0.898853	-1.843004	-1.333273
H	-0.898853	1.843004	-1.333273
H	0.832209	0.000000	23.452157
N	1.529565	0.000000	0.652611
H	1.869275	-0.830502	1.110075
H	1.869275	0.830502	1.110075

8 $SiH_3{-}NH_2 + SiH_4 \longrightarrow SiH_3{-}NH{-}SiH_3 + H_2$

8.1 $SiH_3{-}NH_2 + SiH_4$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	21.241608	0.162575	-0.819325
H	22.719910	0.124301	-0.872483
H	20.825488	0.243256	0.592865
H	20.777097	1.346767	-1.564160
H	20.721283	-1.071380	-1.436974
H	-2.347324	0.962079	-0.205235
H	-2.136279	-0.548893	-0.831385
N	-2.014060	0.029297	-0.013688
Si	-2.322141	-0.657113	1.547526
H	-3.732957	-1.025069	1.815265
H	-1.507664	-1.882150	1.663638
H	-1.913876	0.341608	2.553650

8.2 $SiH_3{-}NH_2 + SiH_4$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.2508198539	0.0480082849	-0.1267917556
H	2.7291217984	0.0097338943	-0.1799495372
H	0.8346995250	0.1286885024	1.2853975827
H	0.7863091019	1.2321998893	-0.8716266149
H	0.7304948951	-1.1859469731	-0.7444405488
H	-2.3473237703	0.9620794271	-0.2052350768
H	-2.1362786488	-0.5488933433	-0.8313847659
N	-2.0140600645	0.0292967117	-0.0136884302
Si	-2.3221414030	-0.6571129240	1.5475257791
H	-3.7329571288	-1.0250694539	1.8152650096
H	-1.5076636893	-1.8821504492	1.6636383833
H	-1.9138760995	0.3416081560	2.5536497726

8.3 transition state

All coordinates are in Ångström units.

Si	0.6525531783	-0.0142223061	-0.0156951762
H	1.3490949405	0.4131832744	-1.2439882127
H	1.2856127444	0.2169141848	1.2972211253
H	0.0600201551	1.6903716209	0.0733902688
H	0.7515193346	-1.5158319508	-0.1323682260
H	-0.9305336271	1.0886884987	-0.0210095299
H	-1.6183896870	-0.4020623306	-0.8970786259
N	-1.2506556851	-0.0551379978	-0.0140807941
Si	-2.1214478831	-0.5991219443	1.4349885319
H	-3.5695127874	-0.5061379852	1.1824892041
H	-1.7496907051	-1.9841099070	1.7674673176
H	-1.7060849431	0.3220740770	2.5046378086

8.4 $SiH_3-NH-SiH_3 + H_2$ **(postreaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.6256808063	-0.1179255206	-0.0471513824
H	0.9637148393	0.8927511593	-1.0711646022
H	1.0540248941	0.3431176432	1.2866089062
H	-1.1089128079	3.2567095211	0.6827109293
H	1.3624831213	-1.3559334098	-0.3864104121
H	-1.2131544702	2.5822707233	0.3997486812
H	-1.5393724072	-0.5322767760	-0.8664597185
N	-1.0909076077	-0.3529584876	0.0226855428
Si	-2.1173531898	-0.5000944897	1.4124268008
H	-3.3675439068	0.2606629285	1.2046102310
H	-2.4942389291	-1.9009740310	1.7069448530
H	-1.3722598767	0.0445648438	2.5628536235

8.5 $SiH_3-NH-SiH_3 + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.625681	-0.117926	-0.047151
H	0.963715	0.892751	-1.071165
H	1.054025	0.343118	1.286609
H	-1.934300	23.074943	3.228585
H	1.362483	-1.355933	-0.386410
H	-2.038541	22.400504	2.945623
H	-1.539372	-0.532277	-0.866460
N	-1.090908	-0.352958	0.022686
Si	-2.117353	-0.500094	1.412427
H	-3.367544	0.260663	1.204610
H	-2.494239	-1.900974	1.706945
H	-1.372260	0.044565	2.562854

9 $(SiH_3)_2NH + SiH_4 \longrightarrow (SiH_3)_3 + H_2$

9.1 $(SiH_3)_2NH + SiH_4$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	21.279744	-0.059883	0.699028
H	20.866688	0.026366	-0.714851
H	22.755554	-0.081142	0.768471
H	20.779771	1.113942	1.439865
H	20.748442	-1.297418	1.301172
H	-2.100669	1.159163	-0.035847
N	-2.088297	0.147954	-0.019221
Si	-2.230174	-0.610127	-1.576355
Si	-2.311005	-0.591332	1.535313
H	-3.624476	-0.962140	-1.929740
H	-3.665860	-0.373082	2.089484
H	-1.438633	-1.856087	-1.568647
H	-2.102982	-2.039930	1.340303
H	-1.714670	0.326871	-2.593540
H	-1.336203	-0.057126	2.507787

9.2 $(SiH_3)_2NH + SiH_4$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.28528191	0.11794927	0.08447058
H	0.87222663	0.20419829	-1.32940839
H	2.76109244	0.09669025	0.15391372
H	0.78530983	1.29177374	0.82530771
H	0.75398055	-1.11958639	0.68661490
H	-2.10066859	1.15916263	-0.03584700
N	-2.08829709	0.14795409	-0.01922104
Si	-2.23017366	-0.61012668	-1.57635508
Si	-2.31100527	-0.59133151	1.53531298
H	-3.62447573	-0.96213979	-1.92973979
H	-3.66586037	-0.37308231	2.08948409
H	-1.43863336	-1.85608656	-1.56864681
H	-2.10298191	-2.03992987	1.34030293
H	-1.71467006	0.32687099	-2.59354047
H	-1.33620334	-0.05712579	2.50778653

9.3 transition state

All coordinates are in Ångström units.

Si	0.5651941371	0.0379410323	0.0275604551
H	1.1359603048	0.1519257406	-1.3304766191
H	1.3597499839	0.5234087547	1.1748096329
H	-0.0158834015	1.7019275507	-0.1226684299
H	0.6298637494	-1.4526452228	0.2654242985
H	-1.0134972591	1.1144547880	-0.0292485209
N	-1.3641438484	-0.0173323337	0.0238034321
Si	-2.0383688473	-0.5343744738	-1.5378062405
Si	-2.1193965540	-0.5529624443	1.5386985644
H	-3.4963622963	-0.6999135797	-1.3821938535
H	-3.4803330749	0.0080856666	1.6096954203
H	-1.4185647344	-1.8099241812	-1.9351041556
H	-2.1866065784	-2.0245527692	1.5700741432
H	-1.7303924991	0.5267285056	-2.5113567730
H	-1.2844610818	-0.0444400338	2.6409796460

9.4 $(SiH_3)_3N + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.5991740526	-0.1834759782	0.0140552044
H	1.0719054672	-0.1469103395	-1.3867221547
H	1.0171180185	1.0511739019	0.7090132510
H	-1.4808454358	3.3138027249	-0.1144384931
H	1.2125820838	-1.3347483318	0.7084516269
H	-1.4106695782	2.5785425673	-0.0989580236
N	-1.1386006766	-0.3212990024	-0.0343781421
Si	-1.9593070177	-0.4586115302	-1.5669641217
Si	-2.0482944304	-0.3983364135	1.4514419868
H	-3.4059563306	-0.5627164170	-1.2781106643
H	-3.0451666495	0.6894012146	1.5235251339
H	-1.5199463401	-1.6589508207	-2.3086041960
H	-2.7601224588	-1.6867797820	1.5820631656
H	-1.7085351802	0.7251781376	-2.4141911119
H	-1.0812658989	-0.2575046115	2.5614187765

9.5 $(SiH_3)_3N + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.599174	-0.183476	0.014055
H	1.071905	-0.146910	-1.386722
H	1.017118	1.051174	0.709013
H	-3.348314	23.218184	-0.557712
H	1.212582	-1.334748	0.708452
H	-3.278138	22.482924	-0.542231
N	-1.138601	-0.321299	-0.034378
Si	-1.959307	-0.458612	-1.566964
Si	-2.048294	-0.398336	1.451442
H	-3.405956	-0.562716	-1.278111
H	-3.045167	0.689401	1.523525
H	-1.519946	-1.658951	-2.308604
H	-2.760122	-1.686780	1.582063
H	-1.708535	0.725178	-2.414191
H	-1.081266	-0.257505	2.561419

10 $(NH_2)_3SiH + NH_2{-}SiH_3 \longrightarrow (NH_2)_3Si{-}NH{-}SiH_3 + H_2$

10.1 $(NH_2)_3SiH + NH_2{-}SiH_3$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.396537	-0.095070	-0.215138
N	-1.327360	1.085980	-1.056229
N	-1.309657	-1.536588	-0.400598
N	1.204420	-0.542801	-0.650856
H	-0.234237	0.496352	1.138092
H	-1.144013	2.064658	-0.899350
H	-2.312853	-1.517911	-0.319676
H	1.968152	0.060297	-0.375574
H	-1.614682	0.923663	-2.009013
H	-0.927070	-2.421777	-0.111978
H	1.389163	-1.003331	-1.528406
H	13.520997	16.186459	7.597414
N	14.174017	16.818585	7.155181
H	15.094022	16.682723	7.547923
Si	13.655297	18.447994	6.867456
H	13.291587	19.228504	8.073374
H	14.765977	19.142498	6.187582
H	12.466459	18.401493	5.992646

10.2 $(NH_2)_3SiH + NH_2{-}SiH_3$ **(prereaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.3965365607	-0.0950699549	-0.2151377635
N	-1.3273598872	1.0859798905	-1.0562286001
N	-1.3096565016	-1.5365875262	-0.4005978875
N	1.2044198430	-0.5428012465	-0.6508561016
H	-0.2342366249	0.4963516386	1.1380918365
H	-1.1440131023	2.0646582230	-0.8993495138
H	-2.3128531670	-1.5179105264	-0.3196757182
H	1.9681520387	0.0602971930	-0.3755744270
H	-1.6146816494	0.9236628057	-2.0090126147
H	-0.9270701792	-2.4217765158	-0.1119780956
H	1.3891628533	-1.0033314584	-1.5284062890
H	1.9647024599	0.9365548649	1.7726552284
N	2.6177218496	1.5686808195	1.3304223923
H	3.5377267178	1.4328189161	1.7231637517
Si	2.0990021910	3.1980900077	1.0426971589
H	1.7352917615	3.9785991159	2.2486155250
H	3.2096822561	3.8925936684	0.3628235981
H	0.9101637892	3.1515889670	0.1678871859

10.3 transition state

All coordinates are in Ångström units.

Si	0.1569185920	0.1072295669	-0.0848498559
N	-0.5689434217	1.5063041091	-0.7649406955
N	-1.2335752480	-0.9567449952	-0.2700953513
N	1.3364687378	-1.0065053992	-0.6500396166
H	-0.0315093441	0.0107164838	1.6345871147
H	-0.0391657252	2.3141433964	-1.0465147993
H	-2.1282438902	-0.5821497160	0.0152049133
H	2.2839946367	-0.7417701150	-0.8568812778
H	-1.4002697530	1.3958879358	-1.3243319657
H	-1.1455254530	-1.8811649387	0.1297890666
H	1.0313944247	-1.7812848560	-1.2176839395
H	0.7582050041	0.5807475134	1.5329551549
N	1.5974596555	1.2309557020	0.7067385305
H	2.5025142723	0.7745909839	0.7414274316
Si	1.6342475676	2.9514947102	0.9887917602
H	2.9190150610	3.3155903722	1.6226407804
H	1.4999473877	3.7301993454	-0.2648653881
H	0.5156740107	3.3269174365	1.8764053988

10.4 $(NH_2)_3Si{-}NH{-}SiH_3 + H_2$ **(postreaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.3373170583	0.2240440281	-0.3068068413
N	-0.4054046978	1.4887552581	-1.2101643733
N	-1.0085108673	-0.5808536261	0.3955221377
N	1.2449544790	-1.0693948810	-0.9889743936
H	0.0816701881	0.2994761002	3.9702599515
H	0.1532103440	2.1859074847	-1.6769770191
H	-1.7593677886	-0.0451558448	0.8008398913
H	2.1619660689	-0.8956435144	-1.3680987537
H	-1.2533419669	1.3057473013	-1.7229624241
H	-0.8708886572	-1.4448538210	0.8947340205
H	0.7726989329	-1.7917660299	-1.5094171367
H	0.1391535378	0.3425446093	3.2344575484
N	1.4884048110	1.1000267151	0.6406798111
H	2.2223753810	0.5569453093	1.0726376435
Si	1.3942526023	2.7586822409	1.1333576847
H	2.5277897146	3.0194743402	2.0470924305
H	1.5004575541	3.6781821341	-0.0218374378
H	0.1320421691	3.0753029874	1.8352657154

10.5 $(NH_2)_3Si{-}NH{-}SiH_3 + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.337317	0.224044	-0.306807
N	-0.405405	1.488755	-1.210164
N	-1.008511	-0.580854	0.395522
N	1.244954	-1.069395	-0.988974
H	-1.035195	0.967354	23.929098
H	0.153210	2.185907	-1.676977
H	-1.759368	-0.045156	0.800840
H	2.161966	-0.895644	-1.368099
H	-1.253342	1.305747	-1.722962
H	-0.870889	-1.444854	0.894734
H	0.772699	-1.791766	-1.509417
H	-0.977711	1.010423	23.193295
N	1.488405	1.100027	0.640680
H	2.222375	0.556945	1.072638
Si	1.394253	2.758682	1.133358
H	2.527790	3.019474	2.047092
H	1.500458	3.678182	-0.021837
H	0.132042	3.075303	1.835266

11 $SiH_3NH_2 \longrightarrow SiHNH_2 + H_2$

11.1 SiH_3NH_2 (reactant)

All coordinates are in Ångström units.

Si	-0.09566652	0.40442850	-1.36249817
H	0.46645314	1.66758556	-1.89906827
H	0.57589808	-0.71119655	-2.05717196
H	-1.54347286	0.40566885	-1.64906393
N	0.10232475	0.15857404	0.33642066
H	-0.42228136	0.72300279	0.98566585
H	1.01820085	-0.03738567	0.70788516

11.2 transition state

All coordinates are in Ångström units.

Si	-0.1614623022	0.5002543922	-1.3331254183
H	1.0141047789	0.9550354440	-2.0952834038
H	0.2739607060	-0.9590988525	-2.0083965433
H	-0.8040578790	-0.6313912646	-2.1152569986
N	0.1637910902	0.1762223119	0.3213727262
H	-0.5189898223	0.3769075983	1.0292778505
H	0.9563574284	-0.3286976292	0.6758107873

11.3 $SiHNH_2 + H_2$ (postreaction complex)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.19099342	0.63455665	-1.29324007
H	1.19855618	0.32942176	-1.82520712
H	0.25451601	-2.17428739	-2.66832744
H	-0.48028637	-2.24959093	-2.68744195
N	0.17888782	0.15977064	0.31221713
H	-0.50755677	0.19957045	1.04980060
H	1.06614840	-0.19191552	0.63734314

11.4 $SiHNH_2 + H_2$ (products)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.190993	0.634557	-1.293240
H	1.198556	0.329422	-1.825207
H	3.075284	-19.958641	-11.374770
H	2.340482	-20.033944	-11.393885
N	0.178888	0.159771	0.312217
H	-0.507557	0.199570	1.049801
H	1.066148	-0.191916	0.637343

12 $(NH_2)_2SiH_2 \longrightarrow (NH_2)_2Si + H_2$

12.1 $(NH_2)_2SiH_2$ (reactant)

All coordinates are in Ångström units.

Si	0.00000000	-0.42733489	-0.08944514
H	0.00000000	-0.95535780	-1.46642280
H	0.00000000	-1.45924627	0.96417348
N	-1.50667892	0.39581746	0.08115192
N	1.50667892	0.39581746	0.08115192
H	-1.84631812	0.67883881	0.98630520
H	1.84631812	0.67883881	0.98630520
H	-1.84624226	1.01517110	-0.63706648
H	1.84624226	1.01517110	-0.63706648

12.2 transition state

All coordinates are in Ångström units.

Si	0.0000000000	-0.4370814716	0.1126347292
H	0.0000000000	-0.8760089710	-1.5067604881
H	0.0000000000	-1.6753407666	-0.7551262263
N	-1.4971011295	0.4089647504	-0.0369968634
N	1.4971011295	0.4089647504	-0.0369968634
H	-2.0716445454	0.5139695674	0.7819680846
H	2.0716445454	0.5139695674	0.7819680846
H	-1.6622544609	1.1502837195	-0.6971234957
H	1.6622544609	1.1502837195	-0.6971234957

12.3 $(NH_2)_2Si + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.34994032	0.99643227
H	0.00000000	-1.34184434	-2.58584340
H	0.00000000	-1.02030680	-3.25102103
N	-1.31664869	0.35468619	-0.11535906
N	1.31664869	0.35468619	-0.11535906
H	-2.26773799	0.35636393	0.21659191
H	2.26773799	0.35636393	0.21659191
H	-1.26923681	0.36308907	-1.12374476
H	1.26923681	0.36308907	-1.12374476

12.4 $(NH_2)_2Si + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.349940	0.996432
H	0.000000	-18.422658	-38.753676
H	0.000000	-18.101121	-39.418854
N	-1.316649	0.354686	-0.115359
N	1.316649	0.354686	-0.115359
H	-2.267738	0.356364	0.216592
H	2.267738	0.356364	0.216592
H	-1.269237	0.363089	-1.123745
H	1.269237	0.363089	-1.123745

13 $NH_2-SiH_3 \longrightarrow SiH_3^{\cdot} + NH_2^{\cdot}$

13.1 NH_2-SiH_3 (minimum)

All coordinates are in Ångström units.

Si	0.60198461	-0.15510285	0.00000000
H	1.08246931	0.53143584	-1.21489514
H	1.08246931	0.53143584	1.21489514
H	1.18156842	-1.52019868	0.00000000
H	-1.63516445	-0.34163777	-0.82622287
H	-1.63516445	-0.34163777	0.82622287
N	-1.12415415	-0.07415816	0.00000000

13.2 $SiH_3^{\cdot} + NH_2^{\cdot}$ (products)

This geometry is used for calculating CASPT2 energy of dissociated fragments. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.601985	-0.155103	0.000000
H	1.082469	0.531436	-1.214895
H	1.082469	0.531436	1.214895
H	1.181568	-1.520199	0.000000
H	-21.615173	0.595295	-0.826223
H	-21.615173	0.595295	0.826223
N	-21.104163	0.862774	0.000000

14 $(NH_2)_2SiH_2 \longrightarrow NH_2{-}SiH_2^{\cdot} + NH_2^{\cdot}$

14.1 $(NH_2)_2SiH_2$ (minimum)

Si	0.000000	0.000000	0.000000
H	-0.678304	-0.578671	1.183564
H	-0.346126	-0.827771	-1.179310
N	-0.526895	1.634972	-0.004945
H	-0.255260	2.276216	-0.732134
H	-1.410248	1.889676	0.405003
N	1.717782	0.000000	0.000000
H	2.246888	0.458096	0.723863
H	2.229978	-0.764266	-0.408407

14.2 $NH_2{-}SiH_2^{\cdot} + NH_2^{\cdot}$ (products)

This geometry is used for calculating CASPT2 energy of dissociated fragments. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.000000	0.000000
H	-0.678304	-0.578671	1.183564
H	-0.346126	-0.827771	-1.179310
N	-0.526895	1.634972	-0.004945
H	-0.255260	2.276216	-0.732134
H	-1.410248	1.889676	0.405003
N	21.720000	0.000000	0.000000
H	22.249106	0.458096	0.723863
H	22.232196	-0.764266	-0.408407

15 $(NH_2)_3SiH \longrightarrow (NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$

15.1 $(NH_2)_3SiH$ **(minimum)**

All coordinates are in Ångström units.

Si	0.000000	0.000000	0.000000
N	-1.515440	0.711147	-0.403986
N	1.515440	0.711147	-0.403986
H	0.000000	-1.277724	-0.747680
H	-1.912900	0.573576	-1.319193
H	1.912900	0.573576	-1.319193
H	-1.794530	1.598484	-0.016355
H	1.794530	1.598484	-0.016355
N	0.000000	0.000000	1.716659
H	-0.833679	-0.245906	2.224533
H	0.833679	-0.245906	2.224533

15.2 $(NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$ **(products)**

This geometry is used for calculating CASPT2 energy of dissociated fragments. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.000000	0.000000
N	-1.515440	0.711147	-0.403986
N	1.515440	0.711147	-0.403986
H	0.000000	-1.277724	-0.747680
H	-1.912900	0.573576	-1.319193
H	1.912900	0.573576	-1.319193
H	-1.794530	1.598484	-0.016355
H	1.794530	1.598484	-0.016355
N	0.000000	0.000000	21.720000
H	-0.833679	-0.245906	22.227874
H	0.833679	-0.245906	22.227874

16 $(NH_2)_4Si \longrightarrow (NH_2)_3Si^{\cdot} + NH_2^{\cdot}$

16.1 $(NH_2)_4Si$ **(minimum)**

All coordinates are in Ångström units.

Si	0.000000	0.000000	0.000000
N	-0.983337	0.000000	-1.414707
N	-0.369776	-1.526848	0.707354
N	-0.369776	1.526848	0.707354
H	-1.326098	-1.841129	0.745207
H	-1.326098	1.841129	0.745207
H	-1.041084	-0.829976	-1.982655
H	-1.041084	0.829976	-1.982655
H	0.144976	-1.841141	1.514206
H	0.144976	1.841141	1.514206
N	1.722890	0.000000	0.000000
H	2.222206	0.829976	-0.276739
H	2.222206	-0.829976	-0.276739

16.2 $(NH_2)_3Si^{\cdot} + NH_2^{\cdot}$ **(products)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.000000	0.000000
N	-0.983337	0.000000	-1.414707
N	-0.369776	-1.526848	0.707354
N	-0.369776	1.526848	0.707354
H	-1.326098	-1.841129	0.745207
H	-1.326098	1.841129	0.745207
H	-1.041084	-0.829976	-1.982655
H	-1.041084	0.829976	-1.982655
H	0.144976	-1.841141	1.514206
H	0.144976	1.841141	1.514206
N	21.720000	0.000000	0.000000
H	22.219316	0.829976	-0.276739
H	22.219316	-0.829976	-0.276739

17 $(SiH_3)_2NH \longrightarrow SiH_3{-}NH^{\cdot} + SiH_3^{\cdot}$

17.1 $(SiH_3)_2NH$ **(minimum)**

All coordinates are in Ångström units.

N	0.000000	0.000000	0.000000
H	1.733716	0.750924	-1.887391
H	-0.888132	0.213585	-0.431466
H	0.946747	-1.497757	-1.985972
Si	1.307491	-0.400391	-1.063286
H	2.429052	-0.825485	-0.201740
Si	0.000000	0.000000	1.732173
H	1.273938	0.565080	2.219959
H	-1.135489	0.823051	2.195031
H	-0.140304	-1.353730	2.313259

17.2 $SiH_3{-}NH^{\cdot} + SiH_3^{\cdot}$ **(products)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	0.000000	0.000000	0.000000
H	1.733716	0.750924	-1.887391
H	-0.888132	0.213585	-0.431466
H	0.946747	-1.497757	-1.985972
Si	1.307491	-0.400391	-1.063286
H	2.429052	-0.825485	-0.201740
Si	0.000000	0.000000	21.730000
H	1.273938	0.565080	22.217786
H	-1.135489	0.823051	22.192858
H	-0.140304	-1.353730	22.311086

18 $(SiH_3)_3N \longrightarrow (SiH_3)_2N^{\cdot} + SiH_3^{\cdot}$

18.1 $(SiH_3)_3N$ (minimum)

All coordinates are in Ångström units.

N	0.000000	0.000000	0.000000
Si	-0.864883	1.513527	0.000000
Si	-0.878311	-1.505774	0.000000
H	-1.722038	1.643285	1.196513
H	-0.562107	-2.312971	1.196513
H	-1.722038	1.643285	-1.196513
H	-0.562107	-2.312971	-1.196513
H	0.145806	2.593256	0.000000
H	-2.318728	-1.170357	0.000000
Si	1.743193	-0.008093	0.000000
H	2.284144	0.669346	-1.196513
H	2.284144	0.669346	1.196513
H	2.172921	-1.423239	0.000000

18.2 $(SiH_3)_2N^{\cdot} + SiH_3^{\cdot}$ (products)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	0.000000	0.000000	0.000000
Si	-0.864883	1.513527	0.000000
Si	-0.878311	-1.505774	0.000000
H	-1.722038	1.643285	1.196513
H	-0.562107	-2.312971	1.196513
H	-1.722038	1.643285	-1.196513
H	-0.562107	-2.312971	-1.196513
H	0.145806	2.593256	0.000000
H	-2.318728	-1.170357	0.000000
Si	21.739766	-0.100930	0.000000
H	22.280717	0.576509	-1.196513
H	22.280717	0.576509	1.196513
H	22.169494	-1.516076	0.000000

19 $NH_3 + SiH_3^{\cdot} \longrightarrow NH_3{-}SiH_3^{\cdot}$

19.1 $NH_3 + SiH_3^{\cdot}$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.093586	0.000000	0.032000
H	0.723770	-1.220002	-0.710351
H	0.723770	1.220002	-0.710351
H	2.560810	0.000000	0.260153
N	-21.956221	0.000000	-0.062159
H	-22.339305	-0.813151	0.404471
H	-22.339305	0.813151	0.404471
H	-22.327349	0.000000	-1.004637

19.2 $NH_3 + SiH^{\cdot}$ (prereaction complex)

All coordinates are in Ångström units.

Si	1.0935863336	0.0000000000	0.0319997512
H	0.7237701797	-1.2200019122	-0.7103511472
H	0.7237701797	1.2200019122	-0.7103511472
H	2.5608104321	0.0000000000	0.2601531826
N	-1.9516764609	0.0000000000	0.0195597993
H	-2.3347597470	-0.8131513998	0.4861902278
H	-2.3347597470	0.8131513998	0.4861902278
H	-2.3228042719	0.0000000000	-0.9229184322

19.3 transition state

All coordinates are in Ångström units.

Si	0.0926221944	-0.0541434119	-1.4597520215
H	-1.1858244027	-0.7368994228	-1.7174756525
H	1.2143234493	-0.7053666512	-2.1463212406
H	0.0504384527	1.3942909191	-1.7190406141
N	-0.0286327009	0.0174902387	0.5049575579
H	0.7946094323	0.5010873450	0.8940490892
H	-0.8826819639	0.5103221924	0.8467036615
H	-0.0348544612	-0.9367812092	0.8951542200

19.4 $NH_2-SiH_3^{\cdot}$ (product)

All coordinates are in Ångström units.

Si	0.0000000000	-0.0000000000	-1.5957883188
H	-1.2724351346	-0.7346407675	-1.7440984477
H	1.2724351346	-0.7346407675	-1.7440984477
H	0.0000000000	1.4692815350	-1.7440984477
N	0.0000000000	-0.0000000000	0.3530758641
H	0.8311683823	0.4798752892	0.7257609327
H	-0.8311683823	0.4798752892	0.7257609327
H	0.0000000000	-0.9597505785	0.7257609327

20 $NH_2-SiH_2^{\cdot} + NH_3 \longrightarrow NH_2-SiH_2-NH_3^{\cdot}$

20.1 $NH_2-SiH_2^{\cdot} + NH_3$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This

geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.341998	0.004498	0.000000
H	-22.855151	1.224904	-0.813709
H	-22.855151	1.224904	0.813709
N	-22.526824	0.719592	0.000000
H	-22.993697	-0.179360	0.000000
H	-0.060855	-0.709475	-1.231892
H	-0.060855	-0.709475	1.231892
N	2.088817	-0.035217	0.000000
H	2.585307	0.265800	-0.825207
H	2.585307	0.265800	0.825207

20.2 $NH_2{-}\dot{S}iH_2 + NH_3$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.34199803	0.00449842	0.00000000
H	-2.86840038	0.59993144	-0.81370890
H	-2.86840038	0.59993144	0.81370890
N	-2.54007384	0.09461893	0.00000000
H	-3.00694620	-0.80433225	0.00000000
H	-0.06085499	-0.70947529	-1.23189175
H	-0.06085499	-0.70947529	1.23189175
N	2.08881660	-0.03521678	0.00000000
H	2.58530683	0.26579995	-0.82520741
H	2.58530683	0.26579995	0.82520741

20.3 transition state

All coordinates are in Ångström units.

Si	0.0978583226	-0.3638325090	0.0000000000
H	-1.8616400392	0.9353073344	-0.8221038211
H	-1.8616400392	0.9353073344	0.8221038211
N	-1.7215365146	0.3319622301	0.0000000000
H	-2.4814320732	-0.3920362365	0.0000000000
H	-0.0165727759	-1.1831145797	-1.2154655340
H	-0.0165727759	-1.1831145797	1.2154655340
N	1.6661771512	0.3625078139	0.0000000000
H	1.9097534773	0.8983928310	-0.8228763706
H	1.9097534773	0.8983928310	0.8228763706

20.4 $NH_2-SiH_2-\dot{N}H_3$ (product)

All coordinates are in Ångström units.

Si	0.09286910	-0.50324681	0.00000000
H	-1.61459529	1.06118469	-0.83635831
H	-1.61459529	1.06118469	0.83635831
N	-1.52154502	0.44393211	0.00000000
H	-2.36236441	-0.17019284	0.00000000
H	0.02507857	-1.29956678	-1.22662146
H	0.02507857	-1.29956678	1.22662146
N	1.45786748	0.50968241	0.00000000
H	1.71589692	1.01861639	-0.83105201
H	1.71589692	1.01861639	0.83105201

21 $(NH_2)_2{-}SiH^{\cdot} + NH_3 \longrightarrow (NH_2)_2{-}SiH{-}NH_3^{\cdot}$

21.1 $(NH_2)_2{-}SiH^{\cdot} + NH_3$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.499484	0.947730	0.529056
H	1.109210	1.186726	1.871545
N	-22.375084	-3.794057	5.206429
H	-22.801894	-4.702819	5.338357
H	-22.586593	-3.248524	6.033285
H	-22.859094	-3.351675	4.434417
N	-0.016435	-0.636937	0.142631
N	1.782184	1.333737	-0.563958
H	0.644607	-1.374255	-0.047498
H	2.423541	2.077910	-0.337270
H	-0.939752	-0.975864	0.389082
H	1.627422	1.278936	-1.558740

21.2 $(NH_2)_2{-}SiH^{\cdot} + NH_3$ **(prereaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.49948423	0.94773015	0.52905579
H	1.10920980	1.18672644	1.87154520
N	-3.02477829	-1.24999084	0.85766813
H	-3.45158827	-2.15875237	0.98959548
H	-3.23628758	-0.70445707	1.68452402
H	-3.50878826	-0.80760892	0.08565615
N	-0.01643461	-0.63693731	0.14263058
N	1.78218381	1.33373707	-0.56395773
H	0.64460661	-1.37425462	-0.04749799
H	2.42354117	2.07790951	-0.33726963
H	-0.93975219	-0.97586365	0.38908222
H	1.62742220	1.27893635	-1.55874003

21.3 transition state

All coordinates are in Ångström units.

Si	-0.1213592751	0.2218179828	0.4566791204
H	0.1959060819	0.3640022831	1.8924968790
N	-2.0141210186	-0.1524533544	0.6799948603
H	-2.2549157858	-1.0561084288	1.1855462417
H	-2.4632009758	0.6191200009	1.1892384638
H	-2.4762909248	-0.1808293749	-0.2362824350
N	0.2138996997	-1.2760833779	-0.3025456633
N	0.9518519263	1.3399228666	-0.3047224906
H	1.1552907710	-1.5034412724	-0.5808990033
H	1.1036234736	2.2160513875	0.1786860996
H	-0.3697430812	-2.0925938004	-0.2163770460
H	0.8209451087	1.5163440877	-1.2910120266

21.4 $(NH_2)_2-SiH-NH_3^{\cdot}$ **(product)**

All coordinates are in Ångström units.

Si	-0.04364244	0.08904553	0.52586551
H	0.32853485	0.24167531	1.93712891
N	-1.90759012	0.08345495	0.57060551
H	-2.29911232	-0.75015997	1.06886585
H	-2.30742664	0.91370740	1.05112549
H	-2.33134254	0.06841699	-0.37901238
N	0.27052613	-1.35276638	-0.30851515
N	0.63792996	1.40016718	-0.30009865
H	1.20503317	-1.58639751	-0.60674143
H	0.86826082	2.25536618	0.18041916
H	-0.32020297	-2.16531047	-0.22426142
H	0.50525875	1.54166986	-1.28817075

22 $NH_3{-}SiH_3^{\cdot} \longrightarrow NH_2SiH_3 + H^{\cdot}$

22.1 $NH_3{-}SiH_3^{\cdot}$ **(reactant)**

All coordinates are in Ångström units.

Si	0.00000000	0.27434706	0.00561423
H	0.00000000	-1.17252398	2.00864365
N	0.00000000	-0.14487456	1.85222289
H	-0.83788164	0.24283873	2.32969095
H	0.83788164	0.24283873	2.32969095
H	-1.23906148	-0.35029197	-0.47371644
H	1.23906148	-0.35029197	-0.47371644
H	0.00000000	1.74236516	0.00120346

22.2 transition state

All coordinates are in Ångström units.

Si	0.0000000000	0.2754518421	0.0458998388
H	0.0000000000	-1.4770523156	2.0174066394
N	0.0000000000	-0.1147325410	1.8008736788
H	0.8228265456	0.1970539019	2.3152905254
H	-0.8228265456	0.1970539019	2.3152905254
H	1.2198665210	-0.3489446221	-0.4856086659
H	-1.2198665210	-0.3489446221	-0.4856086659
H	0.0000000000	1.7192474549	-0.2425988760

22.3 $NH_2SiH_3 + H^{\cdot}$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.27790099	0.05845357
H	0.00000000	-3.31019444	2.32413865
N	0.00000000	0.01070383	1.76584433
H	-0.82612941	0.22338229	2.30224189
H	0.82612941	0.22338229	2.30224189
H	-1.21485032	-0.35327018	-0.49291001
H	1.21485032	-0.35327018	-0.49291001
H	0.00000000	1.69754367	-0.37041027

22.4 $NH_2SiH_3 + H^{\cdot}$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecu-

lar fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.277901	0.058454
H	0.000000	-23.035885	5.640332
N	0.000000	0.010704	1.765844
H	-0.826129	0.223382	2.302242
H	0.826129	0.223382	2.302242
H	-1.214850	-0.353270	-0.492910
H	1.214850	-0.353270	-0.492910
H	0.000000	1.697544	-0.370410

23 $NH_2SiH_2{-}\dot{N}H_3 \longrightarrow (NH_2)_2SiH_2 + H^{\cdot}$

23.1 $NH_2SiH_2{-}\dot{N}H_3$ (reactant)

All coordinates are in Ångström units.

Si	0.00000000	0.27533935	-0.01112733
H	0.00000000	-1.12006512	2.03600637
N	0.00000000	-0.10069085	1.82310557
H	-0.83632344	0.29515796	2.30573553
H	0.83632344	0.29515796	2.30573553
H	-1.22666261	-0.36294862	-0.49196613
H	1.22666261	-0.36294862	-0.49196613
N	0.00000000	1.94031462	-0.35384407
H	-0.83101922	2.49178525	-0.20722350
H	0.83101922	2.49178525	-0.20722350

23.2 transition state

All coordinates are in Ångström units.

Si	0.0000000000	0.3073525378	0.0482040972
H	0.0000000000	-1.4721357433	2.0339646522
N	0.0000000000	-0.1399458274	1.7993476627
H	-0.8203987234	0.1556975985	2.3279289222
H	0.8203987234	0.1556975985	2.3279289222
H	-1.2366881116	-0.3109255697	-0.4446291545
H	1.2366881116	-0.3109255697	-0.4446291545
N	0.0000000000	1.9501866739	-0.4368065070
H	-0.8304535641	2.5150296505	-0.3578287202
H	0.8304535641	2.5150296505	-0.3578287202

23.3 $(NH_2)_2SiH_2 + H^{\cdot}$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.32673722	0.08105323
H	0.00000000	-3.33536967	2.42502702
N	0.00000000	-0.04673719	1.76573653
H	-0.82876084	0.07475721	2.32553411
H	0.82876084	0.07475721	2.32553411
H	-1.24102212	-0.26892101	-0.44808221
H	1.24102212	-0.26892101	-0.44808221
N	0.00000000	1.95632855	-0.48534163
H	-0.82892450	2.52630250	-0.43275787
H	0.82892450	2.52630250	-0.43275787

23.4 $(NH_2)_2SiH_2 + H^{\cdot}$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.326737	0.081053
H	0.000000	-22.941200	6.355517
N	0.000000	-0.046737	1.765737
H	-0.828761	0.074757	2.325534
H	0.828761	0.074757	2.325534
H	-1.241022	-0.268921	-0.448082
H	1.241022	-0.268921	-0.448082
N	0.000000	1.956329	-0.485342
H	-0.828924	2.526302	-0.432758
H	0.828924	2.526302	-0.432758

24 $(NH_2)_2SiH{-}NH_3^{\cdot} \longrightarrow (NH_2)_3SiH + H^{\cdot}$

24.1 $(NH_2)_2SiH{-}NH_3^{\cdot}$ (reactant)

All coordinates are in Ångström units.

Si	0.05438447	0.28188996	-0.01148035
H	0.00619467	-1.15219578	1.99546070
N	-0.01067258	-0.12211522	1.80754513
H	-0.87372235	0.23337708	2.26601388
H	0.78536393	0.27613368	2.34383209
H	1.38923080	-0.17700972	-0.41282997
N	-0.01899826	1.93451109	-0.37126263
H	-0.82977230	2.49480958	-0.16470318
H	0.81885547	2.48921138	-0.44620067
N	-1.34223055	-0.49870518	-0.57161832
H	-1.68075871	-1.35706451	-0.16547286
H	-1.66572585	-0.36704184	-1.51752694

24.2 transition state

All coordinates are in Ångström units.

Si	0.0627955980	0.3122086898	0.0358701549
H	-0.1918061353	-1.4900857024	1.8799953558
N	-0.0241675767	-0.1633993956	1.7724845573
H	-0.8335537798	0.1859726821	2.2829640423
H	0.8062652299	0.0172701811	2.3344610493
H	1.4112370045	-0.1381345611	-0.3502909247
N	-0.0292395686	1.9419826410	-0.4560631076
H	-0.8550757012	2.4998900310	-0.3119682603
H	0.7986727909	2.5078261962	-0.5469927075
N	-1.3333629996	-0.4810219460	-0.5289977232
H	-1.5650902646	-1.3900480479	-0.1515655958
H	-1.6478425976	-0.3700057681	-1.4792538402

24.3 $(NH_2)_3SiH + H^{\cdot}$ **(postreaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.06519609	0.31947518	0.08456127
H	-0.51845998	-3.30136947	1.95415529
N	0.01504213	-0.06165733	1.76355018
H	-0.81003222	0.11958068	2.31320627
H	0.84816599	0.01203667	2.32503818
H	1.41516157	-0.11895068	-0.33611921
N	-0.05146710	1.92661996	-0.52241701
H	-0.88706583	2.47435041	-0.39107714
H	0.76551152	2.51423070	-0.56398405
N	-1.33238729	-0.45345098	-0.54479731
H	-1.58431634	-1.37796987	-0.23598142
H	-1.62226856	-0.28420763	-1.49392708

24.4 $(NH_2)_3SiH + H^{\cdot}$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.065196	0.319475	0.084561
H	-3.762927	-23.003523	3.113311
N	0.015042	-0.061657	1.763550
H	-0.810032	0.119581	2.313206
H	0.848166	0.012037	2.325038
H	1.415162	-0.118951	-0.336119
N	-0.051467	1.926620	-0.522417
H	-0.887066	2.474350	-0.391077
H	0.765512	2.514231	-0.563984
N	-1.332387	-0.453451	-0.544797
H	-1.584316	-1.377970	-0.235981
H	-1.622269	-0.284208	-1.493927

25 $(NH_2)_3SiH{-}\dot{N}H_3^{\cdot} \longrightarrow (NH_2)_4SiH + H^{\cdot}$

25.1 $(NH_2)_3SiH{-}\dot{N}H_3^{\cdot}$ **(reactant)**

All coordinates are in Ångström units.

Si	0.00000000	0.35451001	-0.05311731
H	0.00000000	-1.09726319	1.92997017
N	0.00000000	-0.06181696	1.76467948
H	-0.83185127	0.30525382	2.25794729
H	0.83185127	0.30525382	2.25794729
N	-1.52777465	-0.25047675	-0.49614334
N	1.52777465	-0.25047675	-0.49614334
H	-1.85302458	-1.13882650	-0.14241948
H	1.85302458	-1.13882650	-0.14241948
H	-1.89259714	-0.06798812	-1.41989413
H	1.89259714	-0.06798812	-1.41989413
N	0.00000000	2.00082802	-0.44404931
H	-0.83790665	2.55577406	-0.38223220
H	0.83790665	2.55577406	-0.38223220

25.2 transition state

All coordinates are in Ångström units.

Si	0.0000000000	0.3853811231	-0.0082364458
H	0.0000000000	-1.4594301683	1.7645896574
N	0.0000000000	-0.1001593461	1.7201379250
H	-0.8279469257	0.1468905573	2.2564519803
H	0.8279469257	0.1468905573	2.2564519803
N	-1.5258389789	-0.2396355929	-0.4632149669
N	1.5258389789	-0.2396355929	-0.4632149669
H	-1.7817009718	-1.1593552258	-0.1304952272
H	1.7817009718	-1.1593552258	-0.1304952272
H	-1.8784314384	-0.0818896574	-1.3943609597
H	1.8784314384	-0.0818896574	-1.3943609597
N	0.0000000000	2.0077972184	-0.5339513937
H	-0.8345733374	2.5684965051	-0.4819681978
H	0.8345733374	2.5684965051	-0.4819681978

25.3 $(NH_2)_4SiH + H^{\cdot}$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.38638447	0.04337235
H	0.00000000	-3.24354110	1.64619933
N	0.00000000	0.00104179	1.72288859
H	-0.82984807	0.16200573	2.27091142
H	0.82984807	0.16200573	2.27091142
N	-1.52641807	-0.22112686	-0.47512200
N	1.52641807	-0.22112686	-0.47512200
H	-1.83935821	-1.12344513	-0.15460477
H	1.83935821	-1.12344513	-0.15460477
H	-1.84047141	-0.04447596	-1.41585272
H	1.84047141	-0.04447596	-1.41585272
N	0.00000000	1.98562442	-0.59672739
H	-0.82998408	2.55200432	-0.52551605
H	0.82998408	2.55200432	-0.52551605

25.4 $(NH_2)_4SiH + H^{\cdot}$ **(products)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.386384	0.043372
H	0.000000	-23.242466	1.173503
N	0.000000	0.001042	1.722889
H	-0.829848	0.162006	2.270911
H	0.829848	0.162006	2.270911
N	-1.526418	-0.221127	-0.475122
N	1.526418	-0.221127	-0.475122
H	-1.839358	-1.123445	-0.154605
H	1.839358	-1.123445	-0.154605
H	-1.840471	-0.044476	-1.415853
H	1.840471	-0.044476	-1.415853
N	0.000000	1.985624	-0.596727
H	-0.829984	2.552004	-0.525516
H	0.829984	2.552004	-0.525516

26 $NH_3 + SiH_2 \longrightarrow NH_3{-}SiH_2$

This is a barrierless reaction. Therefore, the transition state is not determined. The only two geometries are reactants ($NH_3{+}SiH_2$) and the product ($NH_3{-}SiH_2$). Geometries of reactants are optimised while placed at great distance where the interaction between them is insignificant.

26.1 $NH_3 + SiH_2$ (reactants)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	16.6273829790	0.0000000000	4.8598619433
H	16.7754743549	-1.0886473814	3.8208916158
H	16.7754743549	1.0886473814	3.8208916158
N	-6.0249678878	0.0000000000	-1.5792952994
H	-6.6548504772	0.0000000000	-0.7870573616
H	-6.2567921618	-0.8123893319	-2.1366802569
H	-6.2567921618	0.8123893319	-2.1366802569

26.2 NH_3-SiH_2 (product)

All coordinates are in Ångström units.

Si	0.8513460658	-0.0729611058	0.3320531249
H	0.9012325635	-1.3372480403	-0.5047469761
H	1.0157640147	0.8506861645	-0.8599971926
N	-1.1575625220	-0.0195317594	0.0134618539
H	-1.6225798405	-0.7354023017	0.5613857369
H	-1.5382264443	0.8760480694	0.2997557923
H	-1.3923328373	-0.1656310266	-0.9621033392

27 $SiH_2-NH_2-SiH_3 \longrightarrow SiH_2 + NH_2-SiH_3$

27.1 $SiH_2 + NH_2-SiH_3$

This geometry is not optimised. This geometry is created by increasing the separation between SiH_2 and NH_2-SiH_3 from the available optimised geometry with the largest $Si-N$ separation (8 Å). This geometry is used in CASPT2 calculation of reactant energies.

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.051034	-0.115225	-2.407392
H	-0.304204	1.138532	-3.143558
H	1.252559	-0.649424	-2.870735
H	-1.081849	-1.123994	-2.720846
N	-0.158660	0.236942	-0.718232
H	0.357101	1.016127	-0.340979
H	-0.174494	-0.521185	-0.054417
H	-20.142225	7.976036	3.005698
Si	-19.736713	9.358351	3.465035
H	-19.622588	9.858838	2.042609

27.2 $SiH_3-NH-SiH_3$ (minimum)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.0919335849	-0.1323518995	-2.4745515976
H	-0.0299706599	1.1217948237	-3.2442424700
H	1.5026367934	-0.5662457581	-2.4231797021
H	-0.6877203435	-1.1704625737	-3.1847615979
N	-0.4534478199	0.1368792382	-0.8503601618
H	-1.4355219171	2.2284709759	0.4885491205
H	0.0697729716	-0.3462598019	-0.1338570847
H	-2.7565824011	0.2434480855	0.4792645623
Si	-1.8238995698	1.0584719622	-0.3279123866
H	-2.5044825635	1.5230184644	-1.5534196821

28 $NH_3-SiH_2 \longrightarrow NH_2-SiH_3$

28.1 NH_3-SiH_2 (reactant)

All coordinates are in Ångström units.

Si	0.9791899536	0.0000000000	0.2557045416
H	1.1109055299	-1.1057026353	-0.7737118433
H	1.1109055299	1.1057026353	-0.7737118433
N	-1.0474273514	0.0000000000	-0.0822162488
H	-1.5751882831	0.0000000000	0.7822576262
H	-1.3174206590	-0.8182012457	-0.6168261944
H	-1.3174206590	0.8182012457	-0.6168261944

28.2 (transition state)

All coordinates are in Ångström units.

Si	0.9020595806	0.0000000000	0.2374121222
H	1.4087314678	-1.1827870305	-0.5076994337
H	1.4087314678	1.1827870305	-0.5076994337
N	-0.9854922472	0.0000000000	-0.1305937219
H	-0.4491597862	0.0000000000	1.1240235316
H	-1.4556397414	-0.8421817252	-0.4362025322
H	-1.4556397414	0.8421817252	-0.4362025322

28.3 NH_2-SiH_3 (product)

All coordinates are in Ångström units.

Si	0.7878120377	0.0000000000	0.2394945804
H	1.4177941136	-1.2148994367	-0.3130769623
H	1.4177941136	1.2148994367	-0.3130769623
N	-0.8695282434	0.0000000000	-0.2494910264
H	1.0264126308	0.0000000000	1.7032289030
H	-1.4294755745	-0.8261932314	-0.1109274012
H	-1.4294755745	0.8261932314	-0.1109274012

29 $\dot{NH_2} + SiH_4 \longrightarrow NH_2SiH_3 + \dot{H}$

29.1 $\dot{NH_2} + SiH_4$ **(reactants)**

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.149731	-0.473562
H	0.000000	0.210443	-1.952571
N	0.000000	-0.908688	22.762345
H	-0.802666	-0.937687	23.394651
H	0.802666	-0.937687	23.394651
H	0.000000	1.527797	0.048366
H	-1.211395	-0.567867	-0.038547
H	1.211395	-0.567867	-0.038547

29.2 $\dot{N}H_2 + SiH_4$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.14973084	-0.47356150
H	0.00000000	0.21044305	-1.95257121
N	0.00000000	0.00151680	2.78024357
H	-0.80266583	-0.02748275	3.41254917
H	0.80266583	-0.02748275	3.41254917
H	0.00000000	1.52779740	0.04836618
H	-1.21139462	-0.56786703	-0.03854744
H	1.21139462	-0.56786703	-0.03854744

29.3 transition state

All coordinates are in Ångström units.

Si	0.0000000000	0.0991153795	-0.0486876296
H	0.0000000000	0.7991659992	-1.3761499895
N	0.0000000000	0.0145545829	1.9889888788
H	-0.8168448707	0.4434567285	2.4224778044
H	0.8168448707	0.4434567285	2.4224778044
H	0.0000000000	1.4442999907	0.7512462671
H	-1.2516247177	-0.6794717046	-0.0882595678
H	1.2516247177	-0.6794717046	-0.0882595678

29.4 $NH_2SiH_3 + H^{\cdot}$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	-0.01697000	0.04278108
H	0.00000000	1.28663664	-0.66520763
N	0.00000000	0.06839829	1.76855150
H	-0.82622162	0.38381543	2.25144779
H	0.82622162	0.38381543	2.25144779
H	0.00000000	3.68369215	1.46862128
H	-1.21508008	-0.74608716	-0.36947257
H	1.21508008	-0.74608716	-0.36947257

29.5 $NH_2SiH_3 + H^{\cdot}$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	-0.016970	0.042781
H	0.000000	1.286637	-0.665208
N	0.000000	0.068398	1.768552
H	-0.826222	0.383815	2.251448
H	0.826222	0.383815	2.251448
H	0.000000	22.350240	8.660716
H	-1.215080	-0.746087	-0.369473
H	1.215080	-0.746087	-0.369473

30 $\dot{N}H_2 + NH_2SiH_3 \longrightarrow (NH_2)_2SiH_2 + \dot{H}$

30.1 $\dot{N}H_2 + NH_2SiH_3$ (reactants)

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.126720	0.295626	-0.495217
H	0.127028	0.599717	-1.942137
N	-1.625267	-3.121052	22.435534
H	-1.938509	-2.241800	22.851869
H	-0.742567	-3.314917	22.912660
H	0.018418	1.555715	0.270736
H	1.445734	-0.295541	-0.157445
N	-1.245601	-0.701013	-0.190010
H	-1.347879	-1.067999	0.744299
H	-1.531036	-1.371111	-0.885408

30.2 $\dot{N}H_2 + NH_2SiH_3$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.12672042	0.29562588	-0.49521699
H	0.12702795	0.59971727	-1.94213693
N	-0.11818540	-0.18198268	2.71021311
H	-0.43142676	0.69726973	3.12654762
H	0.76451529	-0.37584715	3.18733905
H	0.01841808	1.55571487	0.27073645
H	1.44573406	-0.29554114	-0.15744474
N	-1.24560102	-0.70101289	-0.19001020
H	-1.34787906	-1.06799897	0.74429918
H	-1.53103624	-1.37111146	-0.88540819

30.3 transition state

All coordinates are in Ångström units.

Si	0.1218411889	0.2212231790	-0.1110277332
H	0.0966007335	0.8687170292	-1.4593056297
N	-0.0068553565	-0.0397260857	2.0239560603
H	-0.7962317325	0.4438164024	2.4529463385
H	0.8289097399	0.2906984066	2.5063205675
H	0.1077153264	1.4844863901	0.7539070765
H	1.4562815405	-0.4130950633	-0.0327348054
N	-1.3056918902	-0.7348259143	-0.2148036935
H	-1.5105432137	-1.4572540437	0.4541962900
H	-1.7137123363	-0.9161403003	-1.1164694711

30.4 $(NH_2)_2SiH_2 + H^{\cdot}$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.06095177	0.07745945	0.07853941
H	-0.09041513	1.36340063	-0.64230373
N	0.10348465	0.13848159	1.79467547
H	-0.65539110	0.52880441	2.32921327
H	0.98044929	0.21417909	2.28311146
H	0.73397007	3.59819416	1.45454600
H	1.37837088	-0.49849131	-0.27996057
N	-1.33717647	-0.80760340	-0.38237381
H	-1.49089309	-1.75318991	-0.07233158
H	-1.79228748	-0.62533160	-1.26143459

30.5 $(NH_2)_2SiH_2 + H^{\cdot}$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.060952	0.077459	0.078539
H	-0.090415	1.363401	-0.642304
N	0.103485	0.138482	1.794675
H	-0.655391	0.528804	2.329213
H	0.980449	0.214179	2.283111
H	4.239795	21.938082	8.622313
H	1.378371	-0.498491	-0.279961
N	-1.337176	-0.807603	-0.382374
H	-1.490893	-1.753190	-0.072332
H	-1.792287	-0.625332	-1.261435

31 $NH_2^{\cdot} + (NH_2)_2SiH_2 \longrightarrow (NH_2)_3SiH + H^{\cdot}$

31.1 $NH_2^{\cdot} + (NH_2)_2SiH_2$ **(reactants)**

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.265849	-0.437741
H	0.000000	0.802594	-1.814053
N	0.000000	-3.501307	22.373286
H	-0.801088	-2.967010	22.717117
H	0.801088	-2.967010	22.717117
H	0.000000	1.346609	0.569573
H	-1.864731	-1.093420	-1.045293
H	1.864731	-1.093420	-1.045293
N	-1.503522	-0.568328	-0.263967
N	1.503522	-0.568328	-0.263967
H	-1.678856	-1.061576	0.598652
H	1.678856	-1.061576	0.598652

31.2 $\dot{\mathrm{NH}}_2 + (\mathrm{NH}_2)_2\mathrm{SiH}_2$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.26584876	-0.43774095
H	0.00000000	0.80259446	-1.81405305
N	0.00000000	-0.24184903	2.63649015
H	-0.80108838	0.29244764	2.98032141
H	0.80108838	0.29244764	2.98032141
H	0.00000000	1.34660872	0.56957326
H	-1.86473089	-1.09342015	-1.04529291
H	1.86473089	-1.09342015	-1.04529291
N	-1.50352243	-0.56832830	-0.26396693
N	1.50352243	-0.56832830	-0.26396693
H	-1.67885560	-1.06157604	0.59865209
H	1.67885560	-1.06157604	0.59865209

31.3 transition state

All coordinates are in Ångström units.

Si	0.0000000000	0.2251683061	-0.1929319295
H	0.0000000000	0.8698138149	-1.5365490447
N	0.0000000000	-0.1414249621	2.0599733316
H	-0.8120113192	0.2929471590	2.4999643043
H	0.8120113192	0.2929471590	2.4999643043
H	0.0000000000	1.4113669634	0.7431951242
H	-1.9565194221	-0.7952082754	-1.0770610651
H	1.9565194221	-0.7952082754	-1.0770610651
N	-1.5221157242	-0.5878954146	-0.1923737286
N	1.5221157242	-0.5878954146	-0.1923737286
H	-1.7413180887	-1.2869585301	0.4976952486
H	1.7413180887	-1.2869585301	0.4976952486

31.4 $(NH_2)_3SiH + H^{\cdot}$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.04518981	0.06076840
H	0.00000000	1.31025612	-0.70826402
N	0.00000000	0.07461456	1.77712675
H	-0.83365147	0.32890942	2.28085308
H	0.83365147	0.32890942	2.28085308
H	0.00000000	3.65601254	1.58060470
H	-1.91340966	-0.55001200	-1.24815205
H	1.91340966	-0.55001200	-1.24815205
N	-1.51560665	-0.67234094	-0.33094336
N	1.51560665	-0.67234094	-0.33094336
H	-1.79540678	-1.55248366	0.07223247
H	1.79540678	-1.55248366	0.07223247

31.5 $(NH_2)_3SiH + H^{\cdot}$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.045190	0.060768
H	0.000000	1.310256	-0.708264
N	0.000000	0.074615	1.777127
H	-0.833651	0.328909	2.280853
H	0.833651	0.328909	2.280853
H	0.000000	22.091822	9.340446
H	-1.913410	-0.550012	-1.248152
H	1.913410	-0.550012	-1.248152
N	-1.515607	-0.672341	-0.330943
N	1.515607	-0.672341	-0.330943
H	-1.795407	-1.552484	0.072232
H	1.795407	-1.552484	0.072232

32 $\dot{N}H_2 + (NH_2)_3SiH \longrightarrow (NH_2)_4Si + H^{\cdot}$

32.1 $\dot{N}H_2 + (NH_2)_3SiH$ **(reactants)**

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.027780	-0.374960
N	0.000000	-0.431313	22.930519
H	-0.799122	0.180493	23.112077
H	0.799122	0.180493	23.112077
H	0.000000	1.150177	0.593251
H	-1.782601	-1.506062	-0.742441
H	1.782601	-1.506062	-0.742441
N	-1.517112	-0.753653	-0.124375
N	1.517112	-0.753653	-0.124375
H	-1.777983	-0.976866	0.824713
H	1.777983	-0.976866	0.824713
H	-0.831359	0.766352	-2.485227
H	0.831359	0.766352	-2.485227
N	0.000000	0.394889	-2.054920

32.2 $\dot{N}H_2 + (NH_2)_3SiH$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	0.02777992	-0.37495982
N	0.00000000	-0.03738575	2.93312306
H	-0.79912241	0.57442059	3.11468124
H	0.79912241	0.57442059	3.11468124
H	0.00000000	1.15017697	0.59325077
H	-1.78260128	-1.50606229	-0.74244082
H	1.78260128	-1.50606229	-0.74244082
N	-1.51711182	-0.75365346	-0.12437491
N	1.51711182	-0.75365346	-0.12437491
H	-1.77798267	-0.97686562	0.82471329
H	1.77798267	-0.97686562	0.82471329
H	-0.83135920	0.76635156	-2.48522675
H	0.83135920	0.76635156	-2.48522675
N	0.00000000	0.39488859	-2.05491968

32.3 transition state

All coordinates are in Ångström units.

Si	0.0000000000	-0.0018543330	-0.1467732110
N	0.0000000000	0.0241297580	2.1236922253
H	-0.8103379580	0.5300776445	2.4829258905
H	0.8103379580	0.5300776445	2.4829258905
H	0.0000000000	1.3020444345	0.6374907759
H	-1.8795864408	-1.2402987975	-0.8497618535
H	1.8795864408	-1.2402987975	-0.8497618535
N	-1.5359493594	-0.7769079386	-0.0223632323
N	1.5359493594	-0.7769079386	-0.0223632323
H	-1.7738412678	-1.2986046510	0.8048270535
H	1.7738412678	-1.2986046510	0.8048270535
H	-0.8213624293	0.8884707659	-2.2010727342
H	0.8213624293	0.8884707659	-2.2010727342
N	0.0000000000	0.4250790938	-1.8402850384

32.4 $(NH_2)_4Si + H^{\cdot}$ **(postreaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.00000000	-0.22043731	-0.00135292
N	0.00000000	0.40971771	1.60197145
H	-0.83010528	0.84792394	1.96722109
H	0.83010528	0.84792394	1.96722109
H	0.00000000	3.79009793	0.47074004
H	-1.84159691	-1.39837002	-0.96248894
H	1.84159691	-1.39837002	-0.96248894
N	-1.52708195	-1.01323682	-0.08638645
N	1.52708195	-1.01323682	-0.08638645
H	-1.84162965	-1.57522450	0.68814800
H	1.84162965	-1.57522450	0.68814800
H	-0.83000558	1.24194259	-1.69773027
H	0.83000558	1.24194259	-1.69773027
N	0.00000000	0.73578711	-1.43428993

32.5 $(NH_2)_4Si + H^{\cdot}$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	-0.220437	-0.001353
N	0.000000	0.409718	1.601971
H	-0.830105	0.847924	1.967221
H	0.830105	0.847924	1.967221
H	0.000000	23.654720	2.809068
H	-1.841597	-1.398370	-0.962489
H	1.841597	-1.398370	-0.962489
N	-1.527082	-1.013237	-0.086386
N	1.527082	-1.013237	-0.086386
H	-1.841630	-1.575225	0.688148
H	1.841630	-1.575225	0.688148
H	-0.830006	1.241943	-1.697730
H	0.830006	1.241943	-1.697730
N	0.000000	0.735787	-1.434290

33 $SiH_4 + SiH_3^{\cdot} \longrightarrow SiH_3^{\cdot} + SiH_4$

This reaction is symmetric. Reactant and product sides are identical in energy, so only the reactant side is calculated.

33.1 $SiH_4 + SiH_3^{\cdot}$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.000000	0.000000	-23.068767
Si	0.000000	0.000000	2.151233
H	0.000000	0.000000	0.675622
H	-1.216859	-0.702554	-23.519163
H	1.216859	-0.702554	-23.519163
H	0.000000	1.405107	-23.519163
H	1.204404	0.695363	2.643483
H	-1.204404	0.695363	2.643483
H	0.000000	-1.390726	2.643483

33.2 $SiH_4 + SiH_3^{\cdot}$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

SI	0.0000000000	-0.0000000000	-3.0685268815
SI	0.0000000000	0.0000000000	2.1512330406
H	0.0000000000	0.0000000000	0.6756215394
H	-1.2168587221	-0.7025537107	-3.5189229813
H	1.2168587221	-0.7025537107	-3.5189229813
H	0.0000000000	1.4051074215	-3.5189229813
H	1.2044044208	0.6953632165	2.6434834717
H	-1.2044044208	0.6953632165	2.6434834717
H	0.0000000000	-1.3907264331	2.6434834717

33.3 transition state

All coordinates are in Ångström units.

Si	0.0000000000	0.0000000000	-2.1908373685
Si	0.0000000000	-0.0000000000	1.3307184622
H	0.0000000000	-0.0000000000	-0.4300280598
H	-1.2124522744	-0.7000096470	-2.6625824557
H	1.2124522744	-0.7000096470	-2.6625824557
H	0.0000000000	1.4000192941	-2.6625824557
H	1.2124505349	0.7000086427	1.8024724444
H	-1.2124505349	0.7000086427	1.8024724444
H	0.0000000000	-1.4000172854	1.8024724444

34 $\mathrm{NH_2{-}SiH_3 + SiH_3^{\cdot} \longrightarrow NH_2{-}SiH_2^{\cdot} + SiH_4}$

34.1 $\mathrm{NH_2{-}SiH_3 + SiH_3^{\cdot}}$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	-1.760566	-0.940739	0.042283
Si	-1.479453	0.752531	-0.150181
Si	21.546599	-5.623208	1.357948
H	-0.375443	1.118957	-1.073857
H	-2.720440	1.350557	-0.679694
H	-1.145343	1.317478	1.171679
H	21.605771	-4.171592	1.609959
H	22.716072	-6.317008	1.932927
H	21.401834	-5.919804	-0.079659
H	-1.060384	-1.509292	0.492888
H	-2.201978	-1.456329	-0.702650

34.2 $NH_2{-}SiH_3 + \dot{S}iH_3$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	-1.7605662005	-0.9407388506	0.0422831670
Si	-1.4794533171	0.7525305312	-0.1501814082
Si	2.3111442070	-0.2970570805	0.0980900880
H	-0.3754433743	1.1189568026	-1.0738571495
H	-2.7204395933	1.3505571831	-0.6796944383
H	-1.1453430509	1.3174776644	1.1716788483
H	2.3703163445	1.1545596366	0.3501010949
H	3.4806168064	-0.9908566778	0.6730690328
H	2.1663793549	-0.5936528409	-1.3395171809
H	-1.0603841316	-1.5092924131	0.4928876523
H	-2.2019780463	-1.4563294594	-0.7026502214

34.3 transition state

All coordinates are in Ångström units.

N	-1.9928965342	-0.8987200688	0.0457684722
Si	-1.2349744094	0.6516869564	-0.0380626288
Si	2.1842835917	-0.1651227498	-0.0220712598
H	0.5431246446	0.4238063842	-0.0349725631
H	-1.6574504299	1.3019559661	-1.2993180900
H	-1.6519881347	1.4323893776	1.1489739079
H	3.1285845928	0.9718330660	-0.0735867808
H	2.4116240934	-0.9439293416	1.2151080886
H	2.3944106085	-1.0384149727	-1.1979688500
H	-1.9693354081	-1.4278095341	0.9031776707
H	-1.9741768264	-1.5147943939	-0.7515920130

34.4 $NH_2{-}SiH_2^{\cdot} + SiH_4$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	-1.7501857922	-0.9798115357	0.0499451974
Si	-1.5218733039	0.7328381784	0.1351101944
Si	2.3211123602	-0.2033238920	-0.0721539338
H	2.4031971121	1.2674138828	-0.1134738740
H	-1.2336117485	1.2284258082	-1.2311330739
H	-2.7754345820	1.3190181665	0.6633695103
H	3.6150842402	-0.7860229774	-0.4786482802
H	1.9840802214	-0.6542664697	1.2907589057
H	1.2748717599	-0.6629835673	-1.0095149764
H	-2.1635380339	-1.4644236074	0.8315946045
H	-1.0440410845	-1.5518707699	-0.3873495019

34.5 $NH_2{-}\dot{S}iH_2 + SiH_4$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

N	-1.750186	-0.979812	0.049945
Si	-1.521873	0.732838	0.135110
Si	21.725464	-4.930278	-1.118691
H	21.807549	-3.459541	-1.160011
H	-1.233612	1.228426	-1.231133
H	-2.775435	1.319018	0.663370
H	23.019436	-5.512977	-1.525185
H	21.388432	-5.381221	0.244222
H	20.679223	-5.389938	-2.056052
H	-2.163538	-1.464424	0.831595
H	-1.044041	-1.551871	-0.387350

35 $NH_2{-}SiH_2{-}NH_2 + \dot{S}iH_3 \longrightarrow NH_2{-}SiH^{\cdot}{-}NH_2 + SiH_4$

35.1 $NH_2{-}SiH_2{-}NH_2 + \dot{S}iH_3$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.444991	1.610496	-0.217812
Si	0.096989	0.209806	-0.550545
H	-0.042211	0.100792	-2.021320
N	1.244818	-1.002210	-0.152173
H	1.910797	-1.317172	-0.838113
H	1.595436	-1.110792	0.785666
N	-1.315764	-0.087927	0.396580
H	-1.797308	-0.970694	0.314904
H	-1.970316	0.663168	0.553866
H	-1.997109	-2.494743	24.652486
Si	-2.281811	-2.561921	23.200239
H	-1.144734	-1.991016	22.448623
H	-2.529860	-3.960333	22.800521

35.2 $NH_2{-}SiH_2{-}NH_2 + \dot{S}iH_3$ **(prereaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.44499054	1.61049607	-0.21781246
Si	0.09698878	0.20980619	-0.55054528
H	-0.04221059	0.10079164	-2.02132020
N	1.24481841	-1.00220978	-0.15217267
H	1.91079750	-1.31717189	-0.83811331
H	1.59543638	-1.11079191	0.78566635
N	-1.31576385	-0.08792734	0.39657982
H	-1.79730816	-0.97069415	0.31490422
H	-1.97031580	0.66316849	0.55386561
H	-0.01696897	-0.18752562	4.88206372
Si	-0.30167117	-0.25470387	3.42981680
H	0.83540605	0.31620117	2.67820159
H	-0.54971940	-1.65311622	3.03009886

35.3 transition state

All coordinates are in Ångström units.

H	0.1876859732	0.5595284903	1.6531606573
Si	0.1189529447	0.2666313842	-0.1038146746
H	0.2072482904	1.3754942964	-1.0929904316
N	1.3532439914	-0.8327046206	-0.5791280027
H	2.1987913932	-0.4950617956	-1.0107169278
H	1.5158009887	-1.6810570043	-0.0593214798
N	-1.3481843968	-0.6291189647	-0.0249550072
H	-1.6928302797	-1.1508485878	-0.8162818818
H	-2.0991266084	-0.3325934785	0.5776900253
H	0.5911639980	0.7857268139	4.3106048826
Si	-0.0434136479	-0.0353233331	3.2554802883
H	0.4895685161	-1.4139815461	3.3088247261
H	-1.5072801629	-0.0716786540	3.4718428258

35.4 $NH_2{-}SiH^{\cdot}{-}NH_2 + SiH_4$ **(postreaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.32525413	1.05269540	2.69234633
Si	0.05969324	0.26609072	-0.63854105
H	-0.06908715	0.22374597	-2.12359869
N	1.40101836	-0.76118792	-0.29706907
H	2.19080509	-0.78281190	-0.92345704
H	1.68552132	-0.91856524	0.65757321
N	-1.24074335	-0.37157014	0.30281664
H	-1.45211661	-1.35882995	0.26651461
H	-2.07183940	0.17562666	0.46035019
H	0.42974843	-0.07325879	4.81217671
Si	-0.06761339	-0.16654572	3.42241293
H	0.54699775	-1.34975441	2.78778407
H	-1.53406290	-0.30777228	3.44976028

35.5 $NH_2{-}SiH^{\cdot}{-}NH_2 + SiH_4$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-0.298021	-1.065432	22.574206
Si	0.059693	0.266091	-0.638541
H	-0.069087	0.223746	-2.123599
N	1.401018	-0.761188	-0.297069
H	2.190805	-0.782812	-0.923457
H	1.685521	-0.918565	0.657573
N	-1.240743	-0.371570	0.302817
H	-1.452117	-1.358830	0.266515
H	-2.071839	0.175627	0.460350
H	-0.193527	-2.191386	24.694037
Si	-0.690889	-2.284673	23.304273
H	-0.076278	-3.467882	22.669644
H	-2.157338	-2.425899	23.331620

36 $(NH_2)_3SiH + SiH_3^{\cdot} \longrightarrow (NH_2)_3Si^{\cdot} + SiH_4$

36.1 $(NH_2)_3SiH + SiH_3^{\cdot}$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.000000	0.762709	1.794622
Si	0.000000	0.333618	0.376479
N	-1.516778	-0.460591	0.192720
N	1.516778	-0.460591	0.192720
N	0.000000	1.506202	-0.876372
H	-1.899931	-0.996454	0.955201
H	1.899931	-0.996454	0.955201
H	-1.795898	-0.845706	-0.695978
H	1.795898	-0.845706	-0.695978
H	-0.833650	2.033177	-1.078303
H	0.833650	2.033177	-1.078303
Si	0.000000	-10.252630	21.982381
H	0.000000	-11.253005	23.068665
H	-1.220155	-9.424534	22.019309
H	1.220155	-9.424534	22.019309

36.2 $(NH_2)_3SiH + SiH_3^{\cdot}$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.00000000	0.76270911	1.79462191
Si	0.00000000	0.33361780	0.37647947
N	-1.51677810	-0.46059128	0.19271957
N	1.51677810	-0.46059128	0.19271957
N	0.00000000	1.50620218	-0.87637182
H	-1.89993081	-0.99645431	0.95520053
H	1.89993081	-0.99645431	0.95520053
H	-1.79589828	-0.84570569	-0.69597754
H	1.79589828	-0.84570569	-0.69597754
H	-0.83365040	2.03317717	-1.07830339
H	0.83365040	2.03317717	-1.07830339
Si	0.00000000	-1.45178936	4.02038930
H	0.00000000	-2.45216469	5.10667353
H	-1.22015487	-0.62369388	4.05731810
H	1.22015487	-0.62369388	4.05731810

36.3 transition state

All coordinates are in Ångström units.

H	0.0000000000	-0.1773089343	2.2896054774
Si	0.0000000000	0.1616209542	0.5106852637
N	-1.5212216835	-0.5792935527	0.1777929959
N	1.5212216835	-0.5792935527	0.1777929959
N	0.0000000000	1.5477097429	-0.5118905617
H	-1.8893739637	-1.2935555812	0.7854114170
H	1.8893739637	-1.2935555812	0.7854114170
H	-1.8373316140	-0.7117058647	-0.7718628521
H	1.8373316140	-0.7117058647	-0.7718628521
H	-0.8320715459	2.1127414749	-0.5770409234
H	0.8320715459	2.1127414749	-0.5770409234
Si	0.0000000000	-1.1226396706	3.7137923018
H	0.0000000000	-2.5508896944	3.3198568626
H	-1.2105237644	-0.8411366754	4.5157296906
H	1.2105237644	-0.8411366754	4.5157296906

36.4 $(NH_2)_3Si^{\cdot} + SiH_4$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.00000000	0.02809066	4.51199761
Si	0.00000000	0.38923370	0.24491187
N	-1.52269366	-0.41590740	0.10237302
N	1.52269366	-0.41590740	0.10237302
N	0.00000000	1.46040395	-1.10532835
H	-1.88295676	-0.96231989	0.86757855
H	1.88295676	-0.96231989	0.86757855
H	-1.81408010	-0.79577318	-0.78749583
H	1.81408010	-0.79577318	-0.78749583
H	-0.83156217	1.99228538	-1.30910937
H	0.83156217	1.99228538	-1.30910937
Si	0.00000000	-1.43120793	4.30728334
H	0.00000000	-1.72854318	2.85999068
H	-1.20470916	-2.02170980	4.92199275
H	1.20470916	-2.02170980	4.92199275

36.5 $(NH_2)_3Si^{\cdot} + SiH_4$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.000000	-8.150042	22.761753
Si	0.000000	0.389234	0.244912
N	-1.522694	-0.415907	0.102373
N	1.522694	-0.415907	0.102373
N	0.000000	1.460404	-1.105328
H	-1.882957	-0.962320	0.867579
H	1.882957	-0.962320	0.867579
H	-1.814080	-0.795773	-0.787496
H	1.814080	-0.795773	-0.787496
H	-0.831562	1.992285	-1.309109
H	0.831562	1.992285	-1.309109
Si	0.000000	-9.609341	22.557039
H	0.000000	-9.906676	21.109746
H	-1.204709	-10.199843	23.171748
H	1.204709	-10.199843	23.171748

37 $SiH_4 + NH_2^{\cdot} \longrightarrow SiH_3^{\cdot} + NH_3$

37.1 $SiH_4 + NH_2^{\cdot}$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.108998	0.000000	-0.005659
H	0.644175	0.000000	-1.404020
H	0.645203	-1.211480	0.693575
H	0.645203	1.211480	0.693575
H	2.589393	0.000000	-0.005861
N	-22.140958	0.000000	0.039187
H	-22.773827	-0.802744	0.033672
H	-22.773827	0.802744	0.033672

37.2 $SiH_4 + \dot{N}H_2$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.0529915413	-0.0059732390	-2.1002530699
H	-1.1277524164	-0.8199815981	-1.5053166034
H	-0.1971026437	1.4073817423	-1.7083781247
H	-0.1618534873	-0.0942212435	-3.5741685205
H	1.2683538419	-0.5221315038	-1.7009772778
N	0.1980730403	0.2013282720	1.1325947352
H	-0.2264473013	0.8936136210	1.7533722717
H	0.7223532197	-0.4014077129	1.7704025504

37.3 transition state

All coordinates are in Ångström units.

Si	-0.0380826975	0.0066381541	-1.9982041329
H	-0.1802958825	-0.0900566053	-0.4204970042
H	-0.1748824652	1.4183466362	-2.4085626914
H	-1.0949288528	-0.8071340873	-2.6283507706
H	1.2918230346	-0.4978647031	-2.3943024562
N	-0.0618869072	0.0080588968	1.0470709913
H	-0.0339870181	1.0306724288	1.0830855567
H	0.9257267886	-0.2573547202	1.0916695073

37.4 $SiH_3^{\cdot} + NH_3$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	-0.0837340994	-0.0302000962	-2.2791297541
H	-0.7334471426	-0.4972215919	1.1451519399
H	-0.2651733534	1.3620259864	-1.8243290494
H	-0.2002466718	-0.1273647890	-3.7473557360
H	1.2061106962	-0.5750991393	-1.8126350501
N	0.0252082995	0.0769229647	1.4905979552
H	-0.0980016243	0.9999357687	1.0941185889
H	0.8813591365	-0.2998686307	1.1040021454

37.5 $SiH_3^{\cdot} + NH_3$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates

of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.307377	0.000000	-0.035889
H	-22.099129	0.000000	-0.806413
H	0.816692	-1.216252	0.640904
H	0.816692	1.216252	0.640904
H	2.780775	0.000000	-0.123382
N	-22.472012	0.000000	0.134582
H	-22.093611	-0.813677	0.602713
H	-22.093611	0.813677	0.602713

38 $NH_2{-}SiH_3 + \dot{N}H_2 \longrightarrow NH_2{-}Si\dot{H}_2 + NH_3$

38.1 $NH_2SiH_3 + \dot{N}H_2$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.457729	1.572754	-0.516831
Si	0.259988	0.110776	-0.537275
N	0.140407	-2.648619	23.478795
N	-1.192940	-0.222177	0.353946
H	-1.437484	-1.188998	0.516274
H	-2.025832	0.290078	0.101968
H	1.368490	-0.576961	0.151336
H	0.256291	-0.330404	-1.951431
H	0.533992	-1.904210	24.057951
H	0.178166	-2.266245	22.528352

38.2 $NH_2SiH_3 + \dot{N}H_2$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.4577287194	1.5727543982	-0.5168305291
Si	0.2599875348	0.1107759145	-0.5372750882
N	-1.0048130741	-0.5645316724	3.6167102849
N	-1.1929395802	-0.2221766576	0.3539458918
H	-1.4374840073	-1.1889982170	0.5162738164
H	-2.0258318368	0.2900776956	0.1019684513
H	1.3684896370	-0.5769609547	0.1513360324
H	0.2562912691	-0.3304043741	-1.9514309075
H	-0.6112290170	0.1798770844	4.1958657082
H	-0.9670543738	-0.1821580226	2.6662664813

38.3 transition state

All coordinates are in Ångström units.

H	0.1830720585	0.0479147996	1.7030341313
Si	0.0949584861	0.0045248412	0.1195924505
N	-0.0900667991	0.0641001181	3.1556238297
N	-1.4416970860	-0.6462144526	-0.3240776226
H	-1.5395553885	-1.1488866830	-1.1917227574
H	-2.2960720728	-0.1648847998	-0.0944547760
H	1.1200189085	-0.9079906579	-0.4229767294
H	0.3666636755	1.3817087505	-0.3614611963
H	-0.5546705140	0.9761081613	3.1627970296
H	-0.8677281759	-0.5998248086	3.1110612492

38.4 $NH_2SiH_2^{\cdot} + NH_3$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.2896906348	-0.3268345256	2.8923079185
Si	0.1899284174	-0.0410186926	-0.2314077949
N	-0.2381559347	0.1049108508	3.6411349598
N	-1.4480065663	-0.5934794303	-0.2834973441
H	-1.6637697248	-1.4783616600	-0.7158632037
H	-2.0554866459	-0.4265539503	0.5036335352
H	0.7646129016	-0.2148565509	-1.5849246758
H	0.1741775630	1.3861434109	0.1673638974
H	-0.4943549206	1.0327969060	3.3283821141
H	-1.0942085997	-0.4236841937	3.7493361214

38.5 $NH_2SiH_2^{\cdot} + NH_3$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-1.906378	0.421783	22.758417
Si	0.189928	-0.041019	-0.231408
N	-2.434225	0.853528	23.507244
N	-1.448007	-0.593479	-0.283497
H	-1.663770	-1.478362	-0.715863
H	-2.055487	-0.426554	0.503634
H	0.764613	-0.214857	-1.584925
H	0.174178	1.386143	0.167364
H	-2.690424	1.781414	23.194492
H	-3.290277	0.324933	23.615446

39 $NH_2{-}SiH_2{-}NH_2 + NH_2^{\cdot} \longrightarrow NH_2{-}SiH^{\cdot}{-}NH_2 + NH_3$

39.1 $NH_2{-}SiH_2{-}NH_2 + NH_2^{\cdot}$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.953636	0.593725	1.190953
Si	0.355978	0.178514	-0.105243
H	0.082885	1.412604	-0.880917
N	1.362004	-0.735351	-1.158113
H	1.947080	-0.278394	-1.837814
H	1.732768	-1.631585	-0.887851
N	-0.974832	-0.789737	0.358249
H	-1.602984	-1.192121	-0.317321
H	-1.402365	-0.663102	1.265136
H	-8.552098	-0.576756	21.577086
N	-9.536759	-0.852049	21.582802
H	-9.846738	-0.645119	22.533938

39.2 $NH_2{-}SiH_2{-}NH_2 + \dot{N}H_2$ **(prereaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.95363600	0.59372536	1.19095328
Si	0.35597758	0.17851386	-0.10524322
H	0.08288534	1.41260421	-0.88091659
N	1.36200424	-0.73535100	-1.15811290
H	1.94707965	-0.27839390	-1.83781439
H	1.73276775	-1.63158539	-0.88785121
N	-0.97483216	-0.78973726	0.35824943
H	-1.60298381	-1.19212063	-0.31732107
H	-1.40236490	-0.66310189	1.26513617
H	-0.25873422	0.28719459	3.39537618
N	-1.24339443	0.01190134	3.40109237
H	-1.55337341	0.21883182	4.35222854

39.3 transition state

All coordinates are in Ångström units.

H	0.0831652651	0.2295555218	1.6822373833
Si	0.1306676257	0.1219487903	0.0997769744
H	0.1137584510	1.5001818987	-0.4476564094
N	1.4624666432	-0.6248301815	-0.6803587606
H	2.2560332043	-0.0871354093	-0.9883421631
H	1.7020863599	-1.5880046165	-0.5101201399
N	-1.2557831158	-0.8584652726	-0.0885603428
H	-1.6517988552	-1.1125403387	-0.9780121726
H	-1.9233538370	-0.8891862568	0.6660574015
H	0.0856655206	-0.4950439414	3.3894428727
N	-0.6397571839	0.0942025087	2.9733383984
H	-0.3915290779	1.0353242975	3.2882849580

39.4 $NH_2-SiH^{\cdot}-NH_2 + NH_3$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-0.33792362	0.53187834	3.57608277
Si	0.52231945	0.18253044	-0.23595630
H	0.07489387	1.38288030	-1.00333781
N	1.29709998	-0.79044556	-1.43611928
H	1.80995640	-0.34824778	-2.18300382
H	1.71823586	-1.66895156	-1.17667509
N	-0.66730044	-0.79745055	0.50533607
H	-1.27423997	-1.39482574	-0.03431894
H	-1.01296929	-0.60352880	1.43839358
H	-1.22539406	-0.68686924	4.18392756
N	-1.22169645	0.04474055	3.48384954
H	-1.94659794	0.70263521	3.74295755

39.5 $NH_2{-}SiH^{\cdot}{-}NH_2 + NH_3$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-8.822974	-0.138502	21.673819
Si	0.522319	0.182530	-0.235956
H	0.074894	1.382880	-1.003338
N	1.297100	-0.790446	-1.436119
H	1.809956	-0.348248	-2.183004
H	1.718236	-1.668952	-1.176675
N	-0.667300	-0.797451	0.505336
H	-1.274240	-1.394826	-0.034319
H	-1.012969	-0.603529	1.438394
H	-9.710445	-1.357250	22.281664
N	-9.706747	-0.625640	21.581586
H	-10.431648	0.032255	21.840694

40 $(NH_2)_3{-}SiH + NH_2^{\cdot} \longrightarrow (NH_2)_3{-}SiH^{\cdot} + NH_3$

40.1 $(NH_2)_3{-}SiH + NH_2^{\cdot}$ **(reactants)**

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.000000	0.682777	1.925362
Si	0.000000	0.262205	0.503764
N	-1.517119	-0.530849	0.293365
N	1.517119	-0.530849	0.293365
N	0.000000	1.477755	-0.712311
H	-1.780453	-1.227160	0.974769
H	1.780453	-1.227160	0.974769
H	-1.782166	-0.834048	-0.632000
H	1.782166	-0.834048	-0.632000
H	-0.831424	2.022204	-0.875019
H	0.831424	2.022204	-0.875019
N	0.000000	-12.643659	19.938979
H	-0.799104	-12.223684	20.419455
H	0.799104	-12.223684	20.419455

40.2 $(NH_2)_3-SiH + \dot{N}H_2$ **(prereaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.00000000	0.68277725	1.92536181
Si	0.00000000	0.26220518	0.50376432
N	-1.51711861	-0.53084864	0.29336499
N	1.51711861	-0.53084864	0.29336499
N	0.00000000	1.47775541	-0.71231150
H	-1.78045265	-1.22715974	0.97476943
H	1.78045265	-1.22715974	0.97476943
H	-1.78216622	-0.83404804	-0.63199990
H	1.78216622	-0.83404804	-0.63199990
H	-0.83142381	2.02220355	-0.87501903
H	0.83142381	2.02220355	-0.87501903
N	0.00000000	-1.57800707	3.27497887
H	-0.79910440	-1.15803183	3.75545498
H	0.79910440	-1.15803183	3.75545498

40.3 transition state

All coordinates are in Ångström units.

H	0.0000000000	-0.4766064704	2.0121701036
Si	0.0000000000	-0.0719538104	0.4739632184
N	-1.5228289261	-0.6832245529	-0.0417046146
N	1.5228289261	-0.6832245529	-0.0417046146
N	0.0000000000	1.5581471807	-0.0565644670
H	-1.8856112647	-1.5272669139	0.3727769797
H	1.8856112647	-1.5272669139	0.3727769797
H	-1.8295109753	-0.5844457142	-0.9975453516
H	1.8295109753	-0.5844457142	-0.9975453516
H	-0.8345618094	2.1173361901	0.0091911918
H	0.8345618094	2.1173361901	0.0091911918
N	0.0000000000	-1.0282115050	3.3734582355
H	-0.8021729376	-0.4706272066	3.6777757495
H	0.8021729376	-0.4706272066	3.6777757495

40.4 $(NH_2)_3{-}SiH^{\cdot} + NH_3$ **(postreaction complex)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.00000000	-0.39743623	3.40913676
Si	0.00000000	0.39613319	0.47771894
N	-1.52204378	-0.41348779	0.33141048
N	1.52204378	-0.41348779	0.33141048
N	0.00000000	1.50419168	-0.84626689
H	-1.75027896	-1.09936299	1.03532203
H	1.75027896	-1.09936299	1.03532203
H	-1.81331572	-0.73198832	-0.58328132
H	1.81331572	-0.73198832	-0.58328132
H	-0.82948167	2.05059599	-1.01952089
H	0.82948167	2.05059599	-1.01952089
N	0.00000000	-1.41159273	3.42166801
H	-0.81100441	-1.69624768	3.95817810
H	0.81100441	-1.69624768	3.95817810

40.5 $(NH_2)_3{-}SiH^{\cdot} + NH_3$ **(products)**

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.000000	-10.860415	20.448488
Si	0.000000	0.396133	0.477719
N	-1.522044	-0.413488	0.331410
N	1.522044	-0.413488	0.331410
N	0.000000	1.504192	-0.846267
H	-1.750279	-1.099363	1.035322
H	1.750279	-1.099363	1.035322
H	-1.813316	-0.731988	-0.583281
H	1.813316	-0.731988	-0.583281
H	-0.829482	2.050596	-1.019521
H	0.829482	2.050596	-1.019521
N	0.000000	-11.874572	20.461019
H	-0.811004	-12.159227	20.997530
H	0.811004	-12.159227	20.997530

41 $SiH_4 + H^{\cdot} \longrightarrow SiH_3^{\cdot} + H_2$

41.1 $SiH_4 + H^{\cdot}$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.970296	0.000000	0.026410
H	-0.500588	0.000000	-0.084449
H	1.564957	0.000000	-1.323531
H	1.408280	-1.204453	0.756741
H	1.408280	1.204453	0.756741
H	-23.414320	0.000000	-1.828373

41.2 $SiH_4 + H^{\cdot}$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	0.97029566	0.00000000	0.02640966
H	-0.50058752	0.00000000	-0.08444860
H	1.56495739	0.00000000	-1.32353075
H	1.40827967	-1.20445326	0.75674134
H	1.40827967	1.20445326	0.75674134
H	-3.47638717	0.00000000	-0.31093158

41.3 transition state

All coordinates are in Ångström units.

Si	0.9231115241	0.0000000000	0.0228215646
H	-0.6901514980	0.0000000000	-0.0990350416
H	1.4953554373	0.0000000000	-1.3369887079
H	1.3374758898	-1.2115662624	0.7555736231
H	1.3374758898	1.2115662624	0.7555736231
H	-1.7657859748	0.0000000000	-0.1809475382

41.4 $SiH_3^{\cdot} + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.04336995	0.00000000	0.03195783
H	-2.68069857	0.00000000	-0.25003867
H	1.59623187	0.00000000	-1.33589237
H	1.43851995	-1.21709258	0.76626597
H	1.43851995	1.21709258	0.76626597
H	-3.41653282	0.00000000	-0.30604519

41.5 $SiH_3^{\cdot} + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

Si	1.043370	0.000000	0.031958
H	-22.618888	0.000000	-1.759812
H	1.596232	0.000000	-1.335892
H	1.438520	-1.217093	0.766266
H	1.438520	1.217093	0.766266
H	-23.354722	0.000000	-1.815819

42 $NH_2{-}SiH_3 + H^{\cdot} \longrightarrow NH_2{-}\dot{S}iH_2 + H_2$

42.1 $NH_2{-}SiH_3 + H^{\cdot}$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-1.427989	0.959838	0.000000
Si	-0.526625	-0.217636	0.000000
H	-14.387095	19.876669	0.000000
N	1.165099	0.134501	0.000000
H	1.593264	0.520838	-0.826288
H	1.593264	0.520838	0.826288
H	-0.821133	-1.002140	-1.214924
H	-0.821133	-1.002140	1.214924

42.2 $NH_2{-}SiH_3 + H^{\cdot}$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-1.42798929	0.95983810	0.00000000
Si	-0.52662463	-0.21763580	0.00000000
H	-3.08476563	3.37828876	0.00000000
N	1.16509913	0.13450078	0.00000000
H	1.59326434	0.52083781	-0.82628813
H	1.59326434	0.52083781	0.82628813
H	-0.82113324	-1.00214036	-1.21492365
H	-0.82113324	-1.00214036	1.21492365

42.3 transition state

All coordinates are in Ångström units.

H	-1.5018243903	1.1390842173	0.0000000000
Si	-0.5455432879	-0.1809153826	0.0000000000
H	-2.1302063153	2.0167710116	0.0000000000
N	1.1479236690	0.1393520406	0.0000000000
H	1.5907297649	0.5053383988	-0.8279993948
H	1.5907297649	0.5053383988	0.8279993948
H	-0.8770484972	-0.9388862543	-1.2236500041
H	-0.8770484972	-0.9388862543	1.2236500041

42.4 $NH_2-SiH_2^{\cdot} + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-2.64259046	2.81757613	0.00000000
Si	-0.49613544	-0.28963106	0.00000000
H	-3.03114150	3.44537314	0.00000000
N	1.17825834	0.14777040	0.00000000
H	1.58808236	0.55143244	-0.82804315
H	1.58808236	0.55143244	0.82804315
H	-0.75006139	-1.08805779	-1.22169088
H	-0.75006139	-1.08805779	1.22169088

42.5 $NH_2-SiH_2^{\cdot} + H_2$ (product)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-14.011985	19.275905	0.000000
Si	-0.496135	-0.289631	0.000000
H	-14.400536	19.903702	0.000000
N	1.178258	0.147770	0.000000
H	1.588082	0.551432	-0.828043
H	1.588082	0.551432	0.828043
H	-0.750061	-1.088058	-1.221691
H	-0.750061	-1.088058	1.221691

43 $(NH_2)_2SiH_2 + H^{\cdot} \longrightarrow (NH_2)_2SiH^{\cdot} + H_2$

43.1 $NH_2{-}SiH_3 + H^{\cdot}$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.109336	0.292923	1.605178
Si	0.068845	0.125128	0.133653
H	0.044203	1.472498	-0.482800
N	1.420986	-0.630831	-0.608594
H	2.188234	-0.080306	-0.957013
H	1.714693	-1.559317	-0.352616
N	-1.301405	-0.879853	-0.117885
H	-1.607512	-1.135298	-1.042490
H	-2.063060	-0.881428	0.540175
H	-4.879949	-1.642600	23.922509

43.2 $NH_2{-}SiH_3 + H^{\cdot}$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.10933562	0.29292283	1.60517764
Si	0.06884461	0.12512763	0.13365285
H	0.04420349	1.47249794	-0.48279971
N	1.42098631	-0.63083108	-0.60859363
H	2.18823437	-0.08030603	-0.95701294
H	1.71469339	-1.55931686	-0.35261625
N	-1.30140508	-0.87985324	-0.11788529
H	-1.60751250	-1.13529828	-1.04249017
H	-2.06305957	-0.88142768	0.54017510
H	-0.53305227	0.04371752	4.47861224

43.3 transition state

All coordinates are in Ångström units.

H	0.0148554411	0.1940481399	1.8165316758
Si	0.0639209958	0.1150524145	0.1674898759
H	0.0509822224	1.5042755021	-0.3531752199
N	1.4177216549	-0.6167816923	-0.5903781919
H	2.2230177041	-0.0671718781	-0.8437759506
H	1.6651880695	-1.5749905038	-0.4012942958
N	-1.3062411468	-0.8744281702	-0.1157530004
H	-1.6084084453	-1.1302211630	-1.0419741718
H	-2.0581319561	-0.9159716971	0.5522531239
H	-0.1854205396	0.1519180478	2.8384361548

43.4 $(NH_2)_2SiH^{\cdot} + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-0.33270303	0.05527702	3.79376041
Si	0.07344459	0.16624682	0.06614136
H	0.03330919	1.46570306	-0.66380562
N	1.40938075	-0.66397139	-0.64139067
H	2.21631135	-0.14333436	-0.94820854
H	1.67140637	-1.57862687	-0.30787385
N	-1.27505493	-0.88801993	-0.10127615
H	-1.46885434	-1.36572303	-0.96820100
H	-2.09245879	-0.80194002	0.47815716
H	-0.50671350	-0.04609576	4.50419648

43.5 $(NH_2)_2SiH^{\cdot} + H_2$ (products)

This geometry is not optimised. This geometry is created from the postreaction complex (*vide infra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of products energies. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	-2.497917	-0.536314	23.666078
Si	0.073445	0.166247	0.066141
H	0.033309	1.465703	-0.663806
N	1.409381	-0.663971	-0.641391
H	2.216311	-0.143334	-0.948209
H	1.671406	-1.578627	-0.307874
N	-1.275055	-0.888020	-0.101276
H	-1.468854	-1.365723	-0.968201
H	-2.092459	-0.801940	0.478157
H	-2.671928	-0.637687	24.376514

44 $(NH_2)_3SiH + H^{\cdot} \longrightarrow (NH_2)_3Si^{\cdot} + H_2$

44.1 $(NH_2)_3SiH + H^{\cdot}$ (reactants)

This geometry is not optimised. This geometry is created from the prereaction complex (*vide supra*) by increasing the separation between molecular fragments in order to make interaction between them insignificant. This geometry is used in CASPT2 calculation of reactants energy. Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.000000	-0.305926	1.970789
Si	0.000000	-0.051526	0.512629
N	-1.515432	-0.678633	-0.012520
N	1.515432	-0.678633	-0.012520
N	0.000000	1.557347	-0.085917
H	-1.912428	-1.488583	0.435629
H	1.912428	-1.488583	0.435629
H	-1.794521	-0.625026	-0.979359
H	1.794521	-0.625026	-0.979359
H	-0.833680	2.119064	-0.032433
H	0.833680	2.119064	-0.032433
H	0.000000	-12.293008	21.553216

44.2 $(NH_2)_3SiH + H^{\cdot}$ (prereaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.00000000	-0.30592569	1.97078854
Si	0.00000000	-0.05152622	0.51262924
N	-1.51543250	-0.67863317	-0.01252012
N	1.51543250	-0.67863317	-0.01252012
N	0.00000000	1.55734736	-0.08591677
H	-1.91242780	-1.48858281	0.43562880
H	1.91242780	-1.48858281	0.43562880
H	-1.79452068	-0.62502631	-0.97935942
H	1.79452068	-0.62502631	-0.97935942
H	-0.83367958	2.11906407	-0.03243311
H	0.83367958	2.11906407	-0.03243311
H	0.00000000	-1.84955140	4.49249790

44.3 $(NH_2)_3SiH + H^{\cdot}$ (transition state)

All coordinates are in Ångström units.

H	0.0000000000	-0.5188352252	2.1284691195
Si	0.0000000000	-0.0648339102	0.5127887001
N	-1.5211336367	-0.6879329560	0.0087141031
N	1.5211336367	-0.6879329560	0.0087141031
N	0.0000000000	1.5553116235	-0.0492890687
H	-1.9089771504	-1.5056712514	0.4508186028
H	1.9089771504	-1.5056712514	0.4508186028
H	-1.8411331569	-0.5970789811	-0.9434082979
H	1.8411331569	-0.5970789811	-0.9434082979
H	-0.8340371506	2.1151293602	0.0245359235
H	0.8340371506	2.1151293602	0.0245359235
H	0.0000000000	-0.9943638316	3.0151735861

44.4 $(NH_2)_3Si^{\cdot} + H_2$ (postreaction complex)

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.00000000	-1.32883844	3.86331380
Si	0.00000000	-0.04024181	0.49297117
N	-1.52338791	-0.66461075	-0.02825158
N	1.52338791	-0.66461075	-0.02825158
N	0.00000000	1.56202299	-0.13921312
H	-1.90602580	-1.49879140	0.38539962
H	1.90602580	-1.49879140	0.38539962
H	-1.82066427	-0.55837892	-0.98787620
H	1.82066427	-0.55837892	-0.98787620
H	-0.83228936	2.12442514	-0.05762452
H	0.83228936	2.12442514	-0.05762452
H	0.00000000	-1.71813069	4.49120846

44.5 $(NH_2)_3Si^{\cdot} + H_2$ **(products)**

Coordinates of different fragments are shown in different colour. All coordinates are in Ångström units.

H	0.000000	-8.471893	22.546074
Si	0.000000	-0.040242	0.492971
N	-1.523388	-0.664611	-0.028252
N	1.523388	-0.664611	-0.028252
N	0.000000	1.562023	-0.139213
H	-1.906026	-1.498791	0.385400
H	1.906026	-1.498791	0.385400
H	-1.820664	-0.558379	-0.987876
H	1.820664	-0.558379	-0.987876
H	-0.832289	2.124425	-0.057625
H	0.832289	2.124425	-0.057625
H	0.000000	-8.861185	23.173969