Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for:

A theoretical study on the ring expansion of NHCs by silanes

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Computational Details

Geometry optimisations without symmetry constraints were carried out using both M06-2X[1] and B3LYP[2, 3] density functionals. The 6-31G(d) basis set[4, 5] was employed for all atoms. Stationary points were characterised as minima by calculating the Hessian matrix analytically at the same level of theory. All structures are minima with no imaginary frequencies. Thermodynamic corrections were taken from these calculations (standard state of T = 298.15 K and p = 1 atm). Single-point energies were calculated using the TZVP basis set[6, 7] with the MP2 method, at the M06-2X/TZVP optimised geometries. Tabled MP2 energies are presented as ΔG values, which combine the MP2/TZVP electronic energy and M06-2X/TZVP thermochemical correction, defined as MP2/TZVP//M06-2X/6-31G(d). Single point energy calculations were also performed with PBE1PBE[8] and B3LYP DFT, as well as SCS-MP2[9] and SOS-MP2[10] methods, with a TZVP basis set. Transition state optimisations employed the quadratic synchronous transit (QST) approach,[11] while transition states were confirmed as linking reactants and products with intrinsic reaction coordinate (IRC)[12] calculations. All calculations were carried out within Gaussian 09.[13]

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A

NHC^{Me}

M062x/6-31G* optimized geometry (Å).

0 1

6	0.676396	1.211992	-0.000014
7	1.056490	-0.120417	0.000000
6	-0.000001	-0.988107	-0.000014
6	2.433752	-0.568521	0.000007
1	2.416440	-1.657733	0.000092
1	2.958686	-0.211399	-0.891104
1	2.958720	-0.211257	0.891040
7	-1.056491	-0.120415	-0.000003
6	-0.676394	1.211992	0.000000
1	-1.385089	2.026799	0.000034
6	-2.433753	-0.568521	0.000013
1	-2.958678	-0.211388	0.891125
1	-2.958732	-0.211267	-0.891019
1	-2.416439	-1.657732	-0.000061
1	1.385096	2.026796	-0.000046

B1

Ph_2SiH_2

M062x/6-31G* optimized geometry (Å).

0 1

14	0.000000	0.000000	1.558506
1	-1.166609	0.271689	2.439068
1	1.166609	-0.271689	2.439068
6	0.263530	1.520002	0.493013
6	0.952520	1.447106	-0.726215
6	-0.212056	2.770934	0.908752
6	1.164571	2.585090	-1.499426
1	1.319864	0.486367	-1.081515
6	0.000000	3.912936	0.141353
1	-0.760934	2.855190	1.844340
6	0.689647	3.820360	-1.064803
1	1.698732	2.508725	-2.441937
1	-0.376379	4.873075	0.481572
1	0.854436	4.708990	-1.667107
6	-0.263530	-1.520002	0.493013
6	-0.952520	-1.447106	-0.726215
6	0.212056	-2.770934	0.908752
6	-1.164571	-2.585090	-1.499426
1	-1.319864	-0.486367	-1.081515
6	0.000000	-3.912936	0.141353
1	0.760934	-2.855190	1.844340
6	-0.689647	-3.820360	-1.064803
1	-1.698732	-2.508725	-2.441937
1	0.376379	-4.873075	0.481572
1	-0.854436	-4.708990	-1.667107

B2

$PhSiH_3$

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.465956	-0.000284	-0.008512
6	-0.253553	1.201555	-0.007257
6	-0.254839	-1.202576	-0.007205
6	-1.646335	1.204931	0.002411
1	0.278640	2.150113	-0.018346
6	-1.646323	-1.205418	0.002698
1	0.275641	-2.152647	-0.018556
6	-2.343748	0.000464	0.008089
1	-2.186643	2.146912	0.001829
1	-2.187494	-2.146904	0.002545
1	-3.429668	0.000450	0.013097
14	2.339938	-0.000011	0.004402
1	2.877026	-0.258608	1.363902
1	2.857531	-1.056970	-0.899184
1	2.828890	1.325773	-0.448257

B3

Ph_2SiCl_2

M062x/6-31G* optimized geometry (Å).

0 1			
14	-0.049163	0.846737	0.000886
6	1.575777	-0.050100	0.016492
6	2.293171	-0.278157	-1.164927
6	2.069500	-0.575413	1.219780
6	3.476317	-1.011827	-1.144062
1	1.931994	0.128085	-2.106202
6	3.252042	-1.307927	1.240381
1	1.533918	-0.401198	2.150342
6	3.955436	-1.526111	0.057809
1	4.025508	-1.178229	-2.065596
1	3.627486	-1.703502	2.179007
1	4.879666	-2.095791	0.074152
6	-1.519394	-0.285715	-0.015055
6	-1.343310	-1.664389	-0.186696
6	-2.819672	0.219949	0.128678
6	-2.443270	-2.519337	-0.215826
1	-0.341982	-2.074669	-0.295503
6	-3.916465	-0.632455	0.098637
1	-2.974425	1.287658	0.268059
6	-3.727632	-2.003346	-0.073991
1	-2.295813	-3.586843	-0.347614
1	-4.918540	-0.230383	0.210999
1	-4.585278	-2.668974	-0.095497
17	-0.184356	2.061968	1.670066
17	-0.127953	2.083826	-1.655470

B4

Me_2SiH_2

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.000000	0.554565	-0.000003
1	-0.000002	1.434060	1.199932
1	0.000002	1.434050	-1.199945
6	-1.549237	-0.515516	0.000000
1	-2.456307	0.095427	-0.000019
1	-1.576486	-1.159184	-0.884578
1	-1.576504	-1.159153	0.884600
6	1.549237	-0.515516	0.000005
1	1.576496	-1.159173	-0.884580
1	2.456307	0.095427	0.000002
1	1.576495	-1.159163	0.884597

B5

$MeSiH_3$

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.000000	0.000000	0.635438
6	0.000000	0.000000	-1.245410
1	0.000000	-1.021811	-1.635171
1	-0.884914	0.510905	-1.635171
1	0.884914	0.510905	-1.635171
1	0.000000	1.388048	1.160614
1	-1.202085	-0.694024	1.160614
1	1.202085	-0.694024	1.160614

B6

Me_2SiCl_2

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.000000	0.337205	0.000000
6	0.000000	1.337373	1.566628
1	0.000010	0.682715	2.441980
1	0.889037	1.974103	1.610299
1	-0.889048	1.974088	1.610309
6	0.000000	1.337373	-1.566628
1	0.889043	1.974096	-1.610304
1	0.000001	0.682715	-2.441980
1	-0.889043	1.974096	-1.610304
17	1.671805	-0.883269	0.000000
17	-1.671805	-0.883269	0.000000

B7

$SiCl_4$

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.000000	0.000000	0.000000
17	1.172337	1.172337	1.172337
17	-1.172337	-1.172337	1.172337
17	1.172337	-1.172337	-1.172337
17	-1.172337	1.172337	-1.172337

B1

NHC^{Me} + Ph_2SiH_2

Reaction complex C

M062x/6-31G* optimized geometry (Å).

0 1

14	0.090743	-0.215556	-0.025186	1	-0.042978	-0.195915	-1.585544
6	1.900035	-0.859802	-0.141459	1	0.223905	-0.016948	1.522963
6	2.661309	-1.092803	1.011584				
6	2.502000	-1.115748	-1.379515				
6	3.969410	-1.566162	0.936958				
1	2.207521	-0.901454	1.983538				
6	3.810116	-1.587065	-1.468249				
1	1.925078	-0.942543	-2.286051				
6	4.546390	-1.813164	-0.307307				
1	4.538780	-1.747274	1.844912				
1	4.257448	-1.778393	-2.440103				
1	5.566336	-2.182278	-0.371780				
6	-1.541588	-1.210160	0.164059				
6	-2.188694	-1.765507	-0.947591				
6	-2.140030	-1.386659	1.417791				
6	-3.382859	-2.470343	-0.818485				
1	-1.737178	-1.642574	-1.931344				
6	-3.339896	-2.081250	1.559747				
1	-1.646834	-0.971699	2.294781				
6	-3.963413	-2.625364	0.439321				
1	-3.861919	-2.900494	-1.694127				
1	-3.788117	-2.202752	2.542348				
1	-4.897497	-3.170372	0.545200				
6	-0.225589	1.755976	-0.080970				
6	-0.079694	3.952103	0.355749				
6	-1.152162	3.765875	-0.453855				
1	0.341636	4.849230	0.781277				
1	-1.861209	4.465929	-0.866922				
7	0.470966	2.706977	0.572468				
7	-1.216773	2.413438	-0.714408				
6	-2.249578	1.759522	-1.512791				
1	-3.032214	1.362840	-0.862822				
1	-2.667640	2.491242	-2.205249				
1	-1.787608	0.938154	-2.061735				
6	1.622606	2.440273	1.429593				
1	2.196866	3.362320	1.529159				
1	1.284141	2.092744	2.407155				
1	2.241551	1.666780	0.973057				

Reaction complex T1

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.135000	-0.048361	-0.907182
6	-0.357381	1.701138	-0.303767
6	-1.342040	2.442303	-0.974412
6	0.240941	2.287491	0.818270
6	-1.720971	3.709057	-0.541484
1	-1.828130	2.016019	-1.851939
6	-0.131283	3.556396	1.263146
1	1.019265	1.744949	1.354918
6	-1.114898	4.268195	0.583146
1	-2.488018	4.262173	-1.076479
1	0.346275	3.990144	2.137489
1	-1.408490	5.256422	0.925273
6	-1.373503	-1.102247	-0.453535
6	-2.361936	-0.603741	0.406852
6	-1.553731	-2.388960	-0.982616
6	-3.477442	-1.368553	0.745136
1	-2.259939	0.395489	0.822930
6	-2.675528	-3.148964	-0.664767
1	-0.793333	-2.798140	-1.642802
6	-3.637276	-2.641941	0.207513
1	-4.222589	-0.966874	1.425804
1	-2.798647	-4.139308	-1.093824
1	-4.508681	-3.237257	0.464794
6	1.745089	-0.470279	-0.049323
6	3.917005	-1.017889	0.189036
6	3.252945	-1.543983	1.233760
1	4.962728	-1.055307	-0.073964
1	3.600268	-2.133380	2.068021
7	3.013346	-0.239690	-0.535811
7	1.932524	-1.099516	1.159079
6	0.841859	-1.690202	1.900511
1	0.402585	-2.522620	1.334129
1	1.220904	-2.051186	2.858272
1	0.065906	-0.942316	2.081173
6	3.225781	0.163798	-1.904573
1	4.295796	0.290406	-2.076923
1	2.825446	-0.606469	-2.581000
1	2.717369	1.110906	-2.100223
1	1.107804	-1.636076	-1.116726
1	0.366603	0.164207	-2.358613

Reaction complex D

M062x/6-31G* optimized geometry (Å).

0 1			
14	-0.099067	-0.058998	-0.964452
6	0.853323	1.450239	-0.401331
6	0.373823	2.725443	-0.737116
6	2.034332	1.360375	0.348726
6	1.050504	3.876238	-0.343490
1	-0.548314	2.823446	-1.308513
6	2.712780	2.511012	0.744259
1	2.424597	0.385113	0.625456
6	2.224235	3.768023	0.398583
1	0.663754	4.854235	-0.614567
1	3.626600	2.425891	1.325177
1	2.756409	4.663045	0.707896
6	-1.903253	0.076237	-0.456006
6	-2.322493	0.938907	0.566456
6	-2.860695	-0.761095	-1.046894
6	-3.650560	0.960522	0.987196
1	-1.600484	1.600808	1.040002
6	-4.188443	-0.744887	-0.629729
1	-2.566810	-1.435238	-1.849965
6	-4.584346	0.117388	0.390362
1	-3.957207	1.635913	1.780565
1	-4.914726	-1.401432	-1.099898
1	-5.619873	0.133359	0.717401
6	0.654915	-1.654509	-0.240640
6	2.713792	-2.405290	0.426990
6	1.969577	-2.279231	1.525884
1	3.727075	-2.769713	0.325618
1	2.220456	-2.516889	2.550949
7	2.055172	-1.819471	-0.685732
7	0.756359	-1.604535	1.232976
6	-0.426280	-2.100036	1.916933
1	-0.677280	-3.130225	1.609882
1	-0.248866	-2.085497	2.995587
1	-1.280225	-1.453488	1.701015
6	2.184936	-2.519716	-1.949833
1	3.244684	-2.649624	-2.184152
1	1.699669	-3.511063	-1.925423
1	1.730491	-1.927735	-2.748816
1	0.072850	-2.568793	-0.530603
1	-0.063482	-0.195808	-2.448083

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.474341	-1.942676	0.082508
6	2.227422	-1.330760	-1.274316
6	2.756502	-0.868935	-0.113155
1	0.075793	-2.848213	0.552514
1	2.660371	-1.238456	-2.260259
1	3.743605	-0.409547	-0.081174
6	1.289069	-3.550011	-1.548485
1	1.586311	-3.532108	-2.599352
1	2.065919	-4.061209	-0.966945
1	0.341419	-4.085233	-1.461486
6	2.748329	-1.199380	2.273007
1	3.272189	-2.162914	2.299887
1	3.491979	-0.403949	2.428775
1	2.038098	-1.163278	3.104286
7	1.111657	-2.173202	-1.085835
7	2.025309	-0.983924	1.032342
14	-0.037711	-0.290307	0.816054
1	-0.033540	-0.342599	2.305384
6	0.562985	1.340112	0.073553
6	1.646446	2.029932	0.635953
6	-0.103279	1.938539	-1.002586
6	2.055995	3.263441	0.142322
1	2.178991	1.588191	1.475576
6	0.318209	3.162554	-1.521530
1	-0.969261	1.446521	-1.439409
6	1.396670	3.828413	-0.948071
1	2.889870	3.784449	0.604325
1	-0.203680	3.600600	-2.367558
1	1.719622	4.787321	-1.343271
6	-1.920397	-0.254659	0.460356
6	-2.807213	0.377690	1.342744
6	-2.469374	-0.851699	-0.683770
6	-4.177010	0.421012	1.096283
1	-2.418483	0.842756	2.248070
6	-3.838593	-0.814478	-0.943134
1	-1.812054	-1.356782	-1.392209
6	-4.695713	-0.176709	-0.050363
1	-4.842438	0.916254	1.798219
1	-4.237909	-1.283749	-1.838256
1	-5.763935	-0.148190	-0.245309

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.057757	1.929031	-1.298868
6	0.603532	3.184512	0.626279
6	0.415995	2.141008	1.508768
1	0.940625	4.157601	0.946935
1	0.620378	2.364791	2.559638
1	-0.319224	2.062947	-2.348118
6	0.329456	4.310230	-1.473372
1	-0.401915	5.003263	-1.053860
1	1.329615	4.738622	-1.384962
1	0.104654	4.108727	-2.518659
6	-0.193251	0.006326	2.317723
1	0.444243	0.271279	3.170017
1	-1.240034	0.009433	2.639832
1	0.057112	-1.010807	2.004897
7	0.287665	3.050002	-0.711074
7	0.011897	0.923829	1.201443
14	-0.030347	0.115269	-0.664582
6	-1.728076	-0.655631	-0.283671
6	-2.025501	-1.935770	-0.768243
6	-2.738519	0.026218	0.406551
6	-3.264813	-2.529359	-0.544575
1	-1.270854	-2.477684	-1.335495
6	-3.992829	-0.546209	0.611683
1	-2.536493	1.024180	0.793050
6	-4.254793	-1.830936	0.143502
1	-3.463682	-3.530918	-0.915606
1	-4.764771	0.007716	1.139074
1	-5.228044	-2.284331	0.308750
6	1.581063	-0.857156	-0.279852
6	2.528461	-0.521525	0.698180
6	1.862951	-1.979809	-1.074511
6	3.689613	-1.268525	0.882771
1	2.364801	0.347953	1.328844
6	3.004939	-2.752257	-0.880029
1	1.175774	-2.244352	-1.875402
6	3.926510	-2.394887	0.100393
1	4.409636	-0.971341	1.640541
1	3.183433	-3.624504	-1.502914
1	4.827085	-2.984439	0.247679
1	-0.026297	-0.350282	-2.129039

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.354245	-2.121987	-0.867073
6	2.147659	-2.409429	0.662268
6	1.636812	-1.548953	1.576500
1	-0.202209	-2.549477	-1.699403
1	3.096408	-2.901706	0.821030
1	2.227690	-1.388087	2.477745
1	0.474302	-0.609861	-1.845318
6	2.130574	-3.711022	-1.410392
1	2.968772	-3.235159	-1.930741
1	2.500801	-4.556391	-0.825564
1	1.409502	-4.068397	-2.146243
6	0.186496	0.069100	2.576529
1	0.268442	-0.458174	3.533118
1	0.861673	0.936524	2.588584
1	-0.839567	0.436572	2.481830
7	1.474267	-2.752163	-0.529378
7	0.465050	-0.843780	1.474408
14	0.005467	-0.388394	-0.246742
6	0.939552	1.269985	-0.287677
6	0.409673	2.436573	0.284257
6	2.226299	1.348928	-0.839542
6	1.130079	3.630298	0.299956
1	-0.590426	2.418969	0.715594
6	2.961982	2.530032	-0.807265
1	2.654480	0.470336	-1.320217
6	2.411949	3.677722	-0.239993
1	0.689932	4.523237	0.735351
1	3.959065	2.561853	-1.237964
1	2.977246	4.605024	-0.226497
6	-1.841842	-0.111602	-0.269653
6	-2.676365	-0.942757	0.490176
6	-2.430405	0.911016	-1.025189
6	-4.057353	-0.762137	0.493262
1	-2.230794	-1.734321	1.090271
6	-3.810606	1.094922	-1.027994
1	-1.797373	1.572017	-1.613918
6	-4.624570	0.257110	-0.268205
1	-4.690905	-1.412706	1.089294
1	-4.252607	1.891191	-1.619891
1	-5.701267	0.400883	-0.267688

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.740338	-1.513371	-1.280308
6	2.073314	-2.563481	0.454607
6	1.291897	-2.217268	1.488693
1	0.039437	-2.347820	-1.472912
1	2.833328	-3.321265	0.609342
1	1.450091	-2.706261	2.445991
1	0.870282	-0.976704	-2.228515
6	2.702153	-2.811678	-1.850232
1	3.696500	-3.104627	-1.501635
1	2.131238	-3.723195	-2.096808
1	2.820620	-2.222699	-2.764404
6	-0.153623	-0.745289	2.766249
1	-0.362967	-1.571888	3.456494
1	0.607682	-0.097407	3.222627
1	-1.075693	-0.165552	2.653726
7	2.044974	-2.001140	-0.840248
7	0.257421	-1.263278	1.471357
14	-0.000439	-0.350086	0.012866
6	0.879202	1.305788	-0.002859
6	0.269886	2.472067	0.482954
6	2.208127	1.388606	-0.447432
6	0.958162	3.682034	0.518692
1	-0.761295	2.438152	0.830900
6	2.897880	2.597609	-0.417776
1	2.705339	0.489615	-0.809503
6	2.273461	3.745425	0.065172
1	0.469320	4.574958	0.897475
1	3.924697	2.645335	-0.768844
1	2.812269	4.688255	0.089973
6	-1.843454	-0.102183	-0.215294
6	-2.744363	-1.003572	0.370436
6	-2.362597	0.924245	-1.017140
6	-4.116323	-0.882041	0.167452
1	-2.358434	-1.807551	0.994424
6	-3.733639	1.047584	-1.227752
1	-1.686547	1.642060	-1.477896
6	-4.611714	0.144729	-0.632871
1	-4.799821	-1.587213	0.631380
1	-4.117279	1.848902	-1.852423
1	-5.681633	0.241822	-0.792833

B2

NHC^{Me} + $PhSiH_3$

Reaction complex C

M062x/6-31G* optimized geometry (Å).

0 1			
14	-0.641972	0.080142	-0.071552
1	-0.228113	1.485338	0.146488
1	-0.242026	-0.402098	-1.413252
6	-2.534018	0.025490	-0.020409
6	-3.215282	-0.318472	1.154764
6	-3.304573	0.349600	-1.146159
6	-4.607138	-0.329487	1.211448
1	-2.648434	-0.587103	2.044377
6	-4.696050	0.341926	-1.100274
1	-2.809012	0.609275	-2.080327
6	-5.350245	0.002703	0.081891
1	-5.112620	-0.599696	2.134354
1	-5.271286	0.596788	-1.985887
1	-6.435695	-0.006642	0.120913
1	-0.189141	-0.807626	1.024212
6	4.484305	-0.827706	0.032384
6	4.608788	0.511823	0.175590
6	2.376618	0.064113	-0.084126
7	3.129887	-1.070665	-0.122835
7	3.324634	1.024687	0.101544
1	5.480104	1.132557	0.321288
1	5.224801	-1.613468	0.026849
6	3.012572	2.437065	0.204704
1	1.931132	2.541590	0.125663
1	3.348602	2.835023	1.166307
1	3.493345	2.996183	-0.602995
6	2.563441	-2.392510	-0.310165
1	2.787408	-3.031507	0.548602
1	1.483990	-2.280683	-0.406525
1	2.962406	-2.855347	-1.217192

Reaction complex T1

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.117926	-1.261237	-0.465489
1	0.522189	-2.576330	0.086417
1	0.751943	-0.495656	1.137937
6	-1.593679	-0.570863	-0.055462
6	-2.529108	-0.456428	-1.092699
6	-1.992295	-0.193233	1.234119
6	-3.813706	0.030490	-0.857354
1	-2.245747	-0.750646	-2.101029
6	-3.276062	0.286293	1.477627
1	-1.276353	-0.271419	2.048452
6	-4.188432	0.403119	0.430053
1	-4.520565	0.119662	-1.677405
1	-3.567249	0.569961	2.485040
1	-5.188856	0.782691	0.617887
1	-0.097917	-1.561942	-1.937805
6	2.786971	1.745508	0.110027
6	3.578645	0.690386	0.370806
6	1.584579	-0.114478	-0.300019
7	1.595905	1.254428	-0.424533
7	2.886158	-0.461642	-0.005315
1	4.598836	0.642449	0.718480
1	2.975742	2.805217	0.182886
6	3.213794	-1.776860	0.488883
1	2.630173	-1.976393	1.401085
1	2.976020	-2.535826	-0.259388
1	4.280854	-1.816534	0.713018
6	0.382494	2.034420	-0.516441
1	-0.247636	1.654906	-1.323964
1	-0.180619	1.974819	0.424780
1	0.644575	3.072738	-0.727853

Reaction complex D

M062x/6-31G* optimized geometry (Å).

0 1			
14	0.124401	-1.063008	-0.886028
1	0.292930	-2.525861	-0.673893
1	1.258823	-0.311447	1.282129
6	-1.612075	-0.561415	-0.385688
6	-2.378778	0.309782	-1.171527
6	-2.148905	-0.994964	0.835299
6	-3.637307	0.735703	-0.752077
1	-1.985931	0.664567	-2.121748
6	-3.405075	-0.572843	1.259952
1	-1.578287	-1.675068	1.465719
6	-4.150540	0.295314	0.465009
1	-4.217971	1.409643	-1.375071
1	-3.803914	-0.921038	2.208150
1	-5.131039	0.626834	0.793632
1	0.354272	-0.721160	-2.306781
6	2.788569	1.657710	-0.028158
6	3.565132	0.576807	-0.075082
6	1.412004	-0.157009	0.182398
7	1.418349	1.293339	-0.098463
7	2.774697	-0.598900	-0.179607
1	4.642022	0.511639	-0.152810
1	3.070431	2.701734	-0.055526
6	3.233576	-1.740135	0.591584
1	3.193897	-1.548947	1.678227
1	2.613857	-2.612837	0.367451
1	4.263564	-1.975983	0.311539
6	0.516817	2.054271	0.750412
1	-0.519548	1.779668	0.536951
1	0.714359	1.880255	1.822508
1	0.639099	3.119701	0.537664

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	-1.933798	-0.506879	0.814178
6	-1.413983	-0.616754	-1.424575
6	-1.107421	0.694364	-1.254822
1	-1.296595	-1.192442	-2.331851
1	-0.769051	1.310959	-2.086527
1	-2.827292	-0.443723	1.444124
6	-3.478931	-1.641465	-0.681812
1	-4.119721	-0.809043	-0.997627
1	-3.404104	-2.362174	-1.499251
1	-3.914624	-2.141761	0.185274
6	-1.632258	2.629264	0.080290
1	-0.924347	3.271606	-0.464328
1	-2.635656	2.810585	-0.324815
1	-1.618715	2.932174	1.131365
7	-2.135591	-1.169126	-0.346531
7	-1.230360	1.236941	-0.009271
14	-0.294739	0.018043	1.561014
1	-0.025041	-1.054820	2.595730
6	1.315155	-0.078680	0.584464
6	2.063700	-1.260899	0.626972
6	1.844160	1.003118	-0.132928
6	3.279135	-1.374134	-0.046769
1	1.691966	-2.108033	1.199157
6	3.068106	0.908334	-0.786047
1	1.284155	1.934444	-0.179514
6	3.784971	-0.287198	-0.751715
1	3.834329	-2.307176	-0.012828
1	3.464938	1.764338	-1.324790
1	4.737324	-0.366841	-1.268156
1	-0.522568	1.220177	2.407045

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	1.719005	-1.170236	-0.561374
6	2.785562	0.449593	0.855179
6	1.949709	1.494406	0.500660
1	3.611194	0.581262	1.536501
1	2.186960	2.466347	0.942644
1	1.824620	-2.210959	-0.864823
6	3.648118	-1.776429	0.757713
1	4.639653	-1.407893	0.488573
1	3.576608	-1.874002	1.842425
1	3.464396	-2.738082	0.283633
6	0.197606	2.630649	-0.616895
1	0.644460	3.502798	-0.126961
1	0.198384	2.792155	-1.701238
1	-0.846426	2.536458	-0.298233
7	2.638753	-0.801844	0.302908
7	0.922827	1.411072	-0.311786
14	0.233274	-0.240272	-1.345263
1	-0.088429	-1.488721	-2.172076
6	-1.384773	-0.256106	-0.343574
6	-2.529057	-0.807668	-0.936535
6	-1.501120	0.212173	0.971987
6	-3.745786	-0.860985	-0.261872
1	-2.458926	-1.208499	-1.945558
6	-2.708286	0.143321	1.664529
1	-0.629943	0.640530	1.463348
6	-3.836668	-0.387424	1.045003
1	-4.620909	-1.281162	-0.749769
1	-2.769793	0.505712	2.687148
1	-4.781015	-0.436375	1.579829
1	0.286427	0.691884	-2.518525

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

0 1			
6	1.262630	-1.158429	0.244467
6	3.152626	0.111835	-0.441119
6	2.461871	1.264760	-0.581958
1	0.874676	-0.743545	1.896503
1	4.211916	0.067765	-0.651077
1	3.027604	2.135096	-0.910927
1	0.864946	-2.154785	0.437039
6	3.465156	-2.203368	0.280688
1	4.246097	-2.278987	-0.479886
1	3.928395	-2.037453	1.260238
1	2.899059	-3.135500	0.306149
6	0.674684	2.857499	-0.411808
1	1.076769	3.474675	0.403211
1	0.969136	3.303070	-1.368235
1	-0.417062	2.884140	-0.352167
7	2.561950	-1.107751	-0.045935
7	1.122661	1.471910	-0.347783
14	0.272067	0.352212	0.777094
6	-1.483012	-0.062843	0.273895
6	-1.747750	-0.776791	-0.902654
6	-2.569574	0.345869	1.057849
6	-3.052568	-1.078527	-1.282390
1	-0.916577	-1.093688	-1.529617
6	-3.877588	0.041580	0.689118
1	-2.385894	0.906780	1.972082
6	-4.118838	-0.671287	-0.482751
1	-3.241120	-1.628540	-2.199930
1	-4.708376	0.359748	1.312271
1	-5.138142	-0.907981	-0.774437
1	0.101531	1.347338	1.895464

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1

6	1.516302	-0.743649	1.307335
6	2.586336	-0.322700	-0.827598
6	2.253775	0.973372	-0.923879
1	2.375818	-0.446845	1.935784
1	3.386269	-0.709394	-1.449523
1	2.795229	1.607132	-1.620826
1	0.979269	-1.539184	1.836173
6	2.654648	-2.529293	0.121290
1	2.902446	-2.901324	-0.876839
1	3.585571	-2.446202	0.708214
1	2.005196	-3.263599	0.606063
6	0.776800	2.889366	-0.696021
1	1.623393	3.541287	-0.943127
1	0.156592	2.771140	-1.595203
1	0.178785	3.397507	0.067073
7	1.950332	-1.265112	0.011333
7	1.253623	1.619004	-0.178243
14	0.348062	0.706651	0.989842
6	-1.301414	0.106037	0.346028
6	-1.352586	-0.670638	-0.822972
6	-2.504102	0.410005	0.995570
6	-2.568395	-1.129337	-1.320391
1	-0.427128	-0.921160	-1.337712
6	-3.723640	-0.048626	0.501757
1	-2.490547	1.014776	1.900391
6	-3.754927	-0.818304	-0.657906
1	-2.593377	-1.730445	-2.224656
1	-4.646962	0.195440	1.018955
1	-4.703959	-1.176191	-1.046586
1	0.076081	1.539304	2.193134

B3

NHC^{Me} + Me_2SiCl_2

Reaction complex C

M062x/6-31G* optimized geometry (Å).

0 1

14	-0.007162	-0.054791	0.007950	17	-0.127082	0.221528	-2.283823
6	-1.660068	-0.968030	0.090892	17	0.128649	0.205877	2.295487
6	-1.891991	-1.993565	-0.837961				
6	-2.642442	-0.721787	1.060160				
6	-3.058437	-2.750943	-0.794439				
1	-1.154426	-2.197164	-1.608834				
6	-3.827399	-1.454452	1.081903				
1	-2.473268	0.038060	1.817251				
6	-4.034594	-2.475808	0.159320				
1	-3.208277	-3.549816	-1.514403				
1	-4.580521	-1.238333	1.834094				
1	-4.951045	-3.058140	0.186170				
6	1.567364	-1.098961	-0.084348				
6	1.728340	-2.139245	0.842944				
6	2.555296	-0.930626	-1.064734				
6	2.830376	-2.987086	0.785490				
1	0.985384	-2.285513	1.621462				
6	3.677497	-1.755304	-1.100924				
1	2.436723	-0.159519	-1.819845				
6	3.813654	-2.790445	-0.180645				
1	2.925258	-3.795962	1.503673				
1	4.436271	-1.598968	-1.862030				
1	4.680585	-3.443660	-0.218080				
6	0.081188	1.886470	0.004879				
6	-0.446776	4.041792	-0.246699				
6	0.819194	3.982427	0.229507				
1	-1.071588	4.881168	-0.507135				
1	1.525078	4.759289	0.476797				
7	-0.884781	2.741401	-0.377760				
7	1.126605	2.647136	0.378994				
6	2.377394	2.171216	0.967153				
1	2.630083	1.195504	0.553487				
1	3.161201	2.887132	0.715844				
1	2.260152	2.080274	2.047746				
6	-2.177978	2.382038	-0.956775				
1	-2.886959	3.174823	-0.714312				
1	-2.073573	2.264468	-2.036124				
1	-2.523936	1.441632	-0.528327				

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.000464	1.799204	0.049109
6	1.895746	1.972378	-1.247967
6	1.248559	1.070701	-2.013092
1	2.885256	2.373086	-1.416719
1	1.630466	0.733415	-2.972931
6	1.189654	3.979089	-0.053117
1	2.241131	4.264570	-0.115600
1	0.626527	4.496361	-0.837083
1	0.803366	4.260558	0.926132
6	-1.022040	0.459487	-2.549109
1	-1.994020	0.549201	-2.056778
1	-0.946221	1.226413	-3.326986
1	-0.979132	-0.536467	-3.008910
7	1.124484	2.526593	-0.213102
7	0.032163	0.610641	-1.548596
14	-0.024316	-0.036058	0.444531
6	1.573676	-1.030141	0.290952
6	2.471813	-1.152161	1.358433
6	1.879918	-1.719069	-0.894764
6	3.632637	-1.915823	1.243197
1	2.262209	-0.648853	2.296008
6	3.022941	-2.502149	-1.007379
1	1.219891	-1.634097	-1.754554
6	3.909125	-2.597193	0.063710
1	4.316669	-1.982223	2.084045
1	3.226818	-3.032425	-1.933095
1	4.808593	-3.199914	-0.022588
17	-0.161508	0.185727	2.612943
17	-1.454414	2.733820	0.346525
6	-1.645970	-0.938045	0.159022
6	-2.840838	-0.525430	0.762975
6	-1.682399	-2.065760	-0.672542
6	-4.036061	-1.195920	0.516947
1	-2.834263	0.320561	1.444466
6	-2.871438	-2.751154	-0.906360
1	-0.766531	-2.426413	-1.134894
6	-4.053931	-2.309436	-0.319102
1	-4.953028	-0.855123	0.988592
1	-2.873961	-3.630548	-1.543597
1	-4.984771	-2.837706	-0.503492

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.253465	1.914224	-0.173629
6	-1.429847	2.311293	1.426798
6	-1.172428	1.141883	2.090931
1	-2.208131	2.996016	1.722420
1	-1.758079	0.951109	2.991834
6	-0.485251	4.211637	0.224374
1	-1.414430	4.645518	0.589289
1	0.359532	4.617434	0.784616
1	-0.361082	4.426348	-0.836007
6	-0.041168	-0.835834	2.694334
1	0.330851	-0.434649	3.643317
1	-0.972563	-1.386149	2.880359
1	0.701204	-1.533960	2.307394
7	-0.557094	2.753986	0.429140
7	-0.261097	0.237344	1.724113
14	0.013263	-0.008526	-0.194936
6	-1.635049	-0.922046	-0.286754
6	-2.789333	-0.318928	-0.801969
6	-1.744432	-2.216118	0.239720
6	-4.015955	-0.975415	-0.771075
1	-2.721861	0.666608	-1.257804
6	-2.965731	-2.887594	0.248036
1	-0.861738	-2.718576	0.633105
6	-4.106670	-2.263492	-0.247521
1	-4.900904	-0.488290	-1.170670
1	-3.025386	-3.898621	0.641016
1	-5.060828	-2.782033	-0.235633
17	0.079243	0.139102	-2.453317
17	1.612467	2.604400	-0.984598
6	1.633451	-0.935350	-0.012535
6	2.618312	-0.468777	0.867736
6	1.900124	-2.092685	-0.754330
6	3.833603	-1.133339	1.004727
1	2.425054	0.423821	1.460783
6	3.104024	-2.775914	-0.601815
1	1.164203	-2.452442	-1.469639
6	4.074107	-2.294378	0.274129
1	4.589877	-0.748778	1.682797
1	3.291202	-3.677992	-1.176757
1	5.018331	-2.819857	0.383510

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.432349	1.789209	-0.169713
6	-1.284302	2.455607	1.315872
6	-1.188990	1.357526	2.100414
1	-2.055951	3.197075	1.461924
1	-1.912615	1.256670	2.907878
6	-0.190216	4.147264	-0.114665
1	-1.144003	4.650930	0.044846
1	0.591075	4.647015	0.463453
1	0.058491	4.166583	-1.176476
6	-0.337121	-0.729417	2.931158
1	-0.217122	-0.311293	3.935441
1	-1.281819	-1.288965	2.885724
1	0.484575	-1.427151	2.752342
7	-0.335107	2.753355	0.309468
7	-0.290041	0.331012	1.928916
14	-0.003887	-0.020727	0.181372
6	-1.600360	-0.903000	-0.241832
6	-2.751805	-0.278853	-0.741334
6	-1.690605	-2.248825	0.143899
6	-3.950272	-0.975972	-0.847632
1	-2.696868	0.751313	-1.079176
6	-2.887465	-2.953900	0.022725
1	-0.813009	-2.765732	0.530591
6	-4.020840	-2.315654	-0.468851
1	-4.830757	-0.476603	-1.241280
1	-2.930058	-4.000512	0.309829
1	-4.955718	-2.860207	-0.563830
17	-0.208934	0.975322	-2.342228
17	2.042472	2.251521	-0.627309
6	1.513150	-1.078383	0.040614
6	2.556915	-0.928896	0.964301
6	1.650215	-2.021458	-0.985837
6	3.707496	-1.705720	0.870544
1	2.468111	-0.191408	1.760555
6	2.799869	-2.800985	-1.080641
1	0.855902	-2.134225	-1.720242
6	3.826749	-2.643957	-0.152226
1	4.509716	-1.578878	1.591154
1	2.897799	-3.527447	-1.881518
1	4.723953	-3.251412	-0.227754

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.580952	-1.464338	-0.559826
6	1.893828	-2.038441	1.364605
6	1.150536	-1.391890	2.273875
1	2.672829	-2.707612	1.705053
1	1.373858	-1.565428	3.322691
6	2.431406	-3.063278	-0.751115
1	3.444200	-3.180959	-0.360838
1	1.871513	-3.995331	-0.603590
1	2.492420	-2.842962	-1.816209
6	-0.380100	0.263433	3.164304
1	-0.653421	-0.411564	3.983378
1	0.368527	0.977492	3.532270
1	-1.276011	0.821393	2.877777
7	1.797937	-1.945782	-0.051661
7	0.103067	-0.501422	2.022676
14	-0.072058	0.077827	0.393567
6	1.024366	1.548861	0.029714
6	2.375858	1.391034	-0.313848
6	0.535128	2.850991	0.213093
6	3.202651	2.497072	-0.483301
1	2.780485	0.391575	-0.456897
6	1.361150	3.959684	0.046349
1	-0.508102	3.006062	0.482249
6	2.696187	3.782817	-0.305250
1	4.244295	2.356575	-0.756523
1	0.961349	4.959456	0.187314
1	3.342489	4.645351	-0.439678
17	0.735257	-0.997119	-2.296332
17	-0.754915	-2.779853	-0.494597
6	-1.857891	0.437548	0.021608
6	-2.867299	-0.213263	0.746428
6	-2.231054	1.316866	-1.004038
6	-4.209573	0.019715	0.465580
1	-2.591978	-0.917580	1.528759
6	-3.573957	1.546389	-1.292386
1	-1.464932	1.825824	-1.584890
6	-4.562559	0.901417	-0.553909
1	-4.980702	-0.489991	1.035206
1	-3.848426	2.226696	-2.092826
1	-5.610187	1.082668	-0.775790

B4

NHC^{Me} + Me_2SiH_2

Reaction complex T1

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.369247	-0.060445	0.099056
6	2.260120	1.168067	0.122411
6	2.619214	-0.121188	-0.019267
1	-0.196433	-0.080476	-1.587981
1	2.855078	2.066347	0.176702
1	3.592428	-0.576526	-0.116620
6	1.372190	-2.256437	-0.380352
1	2.351094	-2.728990	-0.284790
1	0.645477	-2.809620	0.218282
1	1.049897	-2.263595	-1.431610
6	0.066768	2.378244	0.166929
1	-0.787578	2.329234	0.846186
1	0.664636	3.256373	0.415904
1	-0.295875	2.456556	-0.868355
7	1.462511	-0.891641	0.081580
7	0.879641	1.194724	0.309929
14	-1.419398	-0.545337	-0.272783
1	-1.418582	-1.899248	-0.884658
6	-2.644407	0.703277	-1.004682
1	-2.407239	0.981842	-2.032397
1	-3.640486	0.245340	-0.979703
1	-2.706062	1.611122	-0.395265
6	-2.220595	-0.860602	1.446105
1	-3.239455	-1.255830	1.348366
1	-1.640905	-1.584756	2.031539
1	-2.284699	0.059872	2.041599

Reaction complex D

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.267120	0.021679	-0.490484
6	1.878094	1.122861	0.717093
6	2.315402	-0.121701	0.533254
1	0.466943	0.249060	-1.568343
1	2.369047	1.952100	1.208515
1	3.253901	-0.566116	0.836903
6	1.701716	-1.892911	-1.019742
1	2.475883	-2.545830	-0.607803
1	0.849845	-2.515364	-1.306914
1	2.095657	-1.397479	-1.924223
6	0.199116	2.468523	-0.403244
1	-0.874259	2.509298	-0.606682
1	0.458853	3.328817	0.219485
1	0.739412	2.546766	-1.362708
7	1.288720	-0.936490	-0.009065
7	0.523483	1.244082	0.306867
14	-1.473007	-0.674755	-0.139278
1	-1.610321	-1.939468	-0.918165
6	-2.821341	0.521035	-0.691328
1	-2.676636	0.854002	-1.724200
1	-3.804185	0.042953	-0.629508
1	-2.844636	1.405641	-0.046664
6	-1.575860	-1.018039	1.698782
1	-2.545077	-1.434105	1.989134
1	-0.788904	-1.719084	1.990434
1	-1.414320	-0.086444	2.250027

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.161304	-0.733411	-0.690901
6	-1.505561	-0.337068	1.148285
6	-1.388841	0.972429	0.775876
1	-0.275603	-1.095725	-1.718526
1	-2.052541	-0.715216	2.000159
1	-1.944319	1.748157	1.305189
6	-2.116990	-2.134125	-0.357172
1	-2.579339	-2.655580	0.483896
1	-2.888822	-1.567478	-0.891803
1	-1.665141	-2.872823	-1.022302
6	-0.976983	2.445582	-1.068682
1	-1.938527	2.324573	-1.585547
1	-1.043036	3.345749	-0.440472
1	-0.200798	2.619787	-1.819937
7	-1.080020	-1.239130	0.155390
7	-0.605886	1.291296	-0.273028
14	1.445058	0.129117	-0.239364
6	1.682138	0.621225	1.561424
1	1.350783	-0.187412	2.220926
1	2.751534	0.773364	1.743617
1	1.140775	1.528050	1.833209
6	2.791400	-1.196202	-0.524120
1	3.794869	-0.772907	-0.398308
1	2.692940	-2.023430	0.188773
1	2.741768	-1.621533	-1.533127
1	1.742827	1.169047	-1.259439

Reaction complex T2a

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.742195	-0.973123	-0.489241
6	-1.722081	0.992318	0.481420
6	-0.634124	1.814813	0.211423
1	-1.040659	-1.920170	-0.939356
1	-2.642338	1.375315	0.894275
1	-0.764651	2.879362	0.433701
6	-3.121334	-0.865419	-0.080664
1	-3.581416	-0.777038	0.905123
1	-3.713357	-0.308173	-0.809186
1	-3.059209	-1.915062	-0.361283
6	1.482840	2.374866	-0.695186
1	1.124875	3.402579	-0.557612
1	2.397812	2.240907	-0.104407
1	1.756509	2.235809	-1.747062
7	-1.765326	-0.291222	-0.019068
7	0.486144	1.396727	-0.317289
14	1.124923	-0.637859	-0.219792
6	1.598187	-0.258713	1.582315
1	0.684268	-0.068160	2.159214
1	2.132435	-1.089321	2.052130
1	2.212783	0.643474	1.664647
6	1.574962	-2.518778	-0.314932
1	2.655246	-2.648266	-0.170752
1	1.071678	-3.120166	0.453969
1	1.329640	-2.959893	-1.290571
1	2.024211	-0.175493	-1.322067

Reaction complex T2b

M062x/6-31G* optimized geometry (Å).

0 1			
6	1.031158	0.736354	-0.656637
6	1.585976	-1.135275	0.675299
6	0.352968	-1.692498	0.500533
1	1.476908	1.545655	-1.243188
1	2.365342	-1.597651	1.261336
1	0.194064	-2.671468	0.958177
6	3.367772	0.314066	-0.092638
1	3.751350	0.432204	0.923469
1	3.883384	-0.516979	-0.578709
1	3.524556	1.235014	-0.652335
6	-1.770475	-2.085873	-0.457124
1	-1.388154	-3.067856	-0.754639
1	-2.422162	-2.209406	0.417260
1	-2.375405	-1.698077	-1.279790
7	1.929138	0.023712	-0.031162
7	-0.663576	-1.168257	-0.202531
14	-0.946858	0.737370	-0.382445
6	-2.645357	0.551843	0.546835
1	-2.483470	0.230700	1.585543
1	-3.145752	1.525075	0.588775
1	-3.350654	-0.154789	0.099984
6	-0.659472	2.500701	0.423691
1	-1.542445	3.122865	0.239247
1	-0.577458	2.388566	1.513474
1	0.219364	3.063165	0.090544
1	-1.307802	0.925708	-1.818821

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	-1.085352	-0.788272	-0.744214
6	-1.623305	1.050978	0.619967
6	-0.369344	1.567373	0.542533
1	-1.529671	-1.561653	-1.384115
1	-2.412592	1.536535	1.174189
1	-0.218983	2.518680	1.054473
6	-3.439043	-0.281849	-0.285669
1	-3.873225	-0.424064	0.706978
1	-3.894005	0.593208	-0.755457
1	-3.612525	-1.168632	-0.893758
6	1.828580	1.990372	-0.248811
1	1.462875	3.021332	-0.239108
1	2.574772	1.868982	0.543479
1	2.324398	1.824375	-1.206959
7	-1.992239	-0.067756	-0.150266
7	0.705970	1.061351	-0.104683
14	0.962215	-0.770116	-0.368643
6	2.883958	-0.699248	-0.091421
1	3.189625	-0.325363	0.895070
1	3.216916	-1.744481	-0.153279
1	3.453331	-0.148791	-0.849692
6	0.545926	-1.902929	1.120708
1	1.442609	-2.292369	1.612053
1	-0.022213	-1.326244	1.862910
1	-0.082972	-2.752729	0.830462
1	1.066021	-1.410876	-1.730150

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

0 1			
6	-1.018290	-1.010370	-0.390867
6	-1.621376	1.234513	0.096229
6	-0.369514	1.716512	-0.100320
1	-1.374425	-1.990809	-0.704480
1	-2.435228	1.879114	0.395688
1	-0.231991	2.787291	0.053025
6	-3.357024	-0.489543	0.091301
1	-3.587890	-0.507825	1.161772
1	-4.010017	0.231561	-0.406471
1	-3.526609	-1.481867	-0.327957
6	1.977852	1.754258	-0.531902
1	1.883582	2.564299	-1.263870
1	2.280797	2.190161	0.432225
1	2.781659	1.093234	-0.869400
7	-1.962536	-0.118846	-0.118327
7	0.739985	0.994889	-0.446437
14	0.764253	-0.752993	0.156148
6	1.825806	-1.771035	-1.013196
1	2.827014	-1.943170	-0.607053
1	1.369095	-2.747617	-1.201658
1	1.923315	-1.253484	-1.973138
6	1.667638	-0.378444	1.793072
1	1.932611	-1.299711	2.319538
1	2.580964	0.212675	1.648226
1	1.004810	0.198190	2.450417
1	-0.189926	-1.857790	0.994512

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.956774	-1.020084	-0.541771
6	-1.605537	1.243418	0.027105
6	-0.388059	1.794612	-0.086291
1	-1.072577	-0.923680	-1.638550
1	-2.474383	1.892444	0.036140
1	-0.307810	2.875207	-0.168712
1	-1.204899	-2.056889	-0.281716
6	-3.267156	-0.483968	-0.044274
1	-3.909423	0.164916	0.557998
1	-3.567316	-0.393136	-1.102980
1	-3.435191	-1.517294	0.272881
6	2.028958	1.894026	0.084520
1	2.041786	2.753327	-0.598042
1	2.117042	2.274406	1.112188
1	2.917311	1.292191	-0.131710
7	-1.875468	-0.135821	0.172979
7	0.832459	1.099218	-0.115705
14	0.818522	-0.640873	-0.015291
6	2.079603	-1.379612	-1.196878
1	3.103938	-1.105829	-0.922376
1	2.024237	-2.473709	-1.184537
1	1.901878	-1.039513	-2.221479
6	1.131098	-1.269457	1.726230
1	1.177424	-2.363685	1.758202
1	2.074545	-0.883900	2.127927
1	0.322395	-0.940017	2.386074

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NHC^{Me} + $MeSiH_3$

Reaction complex T1

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.191950	-0.091746	-0.255297
6	-1.830995	1.402123	0.147179
6	-2.381672	0.175787	0.199274
1	0.565732	-0.425667	1.302742
1	-2.267208	2.379506	0.282568
1	-3.396769	-0.134298	0.392666
6	-1.479494	-2.151794	0.138446
1	-2.528970	-2.448865	0.168697
1	-0.962829	-2.734646	-0.626229
1	-1.006647	-2.337217	1.114342
6	0.512210	2.255307	-0.086849
1	1.256469	2.169398	-0.881835
1	0.049699	3.242028	-0.143052
1	1.004284	2.129210	0.888969
7	-1.399021	-0.743026	-0.165972
7	-0.504204	1.244362	-0.250605
14	1.518735	-0.872377	-0.242790
1	1.357008	-2.297739	0.131628
1	1.940869	-0.965807	-1.703979
6	3.034058	0.009453	0.462875
1	3.919405	-0.553740	0.144448
1	3.142954	1.020291	0.057898
1	3.013343	0.066695	1.552469

Reaction complex D

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.083341	-0.127545	0.288070
6	-1.649129	1.357807	-0.485283
6	-2.232659	0.161277	-0.452749
1	-0.118790	-0.082506	1.406678
1	-2.070554	2.315083	-0.761101
1	-3.252364	-0.105909	-0.695715
6	-1.702844	-1.921956	0.689129
1	-2.608274	-2.385210	0.288307
1	-0.925541	-2.689069	0.745139
1	-1.910352	-1.555660	1.709729
6	0.313912	2.266154	0.612062
1	1.396961	2.135264	0.685383
1	0.121209	3.251049	0.178292
1	-0.111625	2.234227	1.630163
7	-1.276509	-0.855031	-0.197749
7	-0.252565	1.241995	-0.247926
14	1.492560	-0.946655	-0.394774
1	1.554459	-2.339150	0.130143
1	1.373726	-0.998052	-1.869099
6	3.055326	-0.023864	0.109889
1	3.944599	-0.590776	-0.181738
1	3.109008	0.953344	-0.379148
1	3.097637	0.130557	1.192810

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.112382	-0.613248	-0.616674
6	-1.417857	-0.511364	1.104601
6	-1.334588	0.834286	0.901634
1	-2.012477	-1.012709	1.854792
1	-1.958235	1.525987	1.467892
1	1.955740	1.436679	-0.739050
6	-1.799475	-2.110171	-0.676584
1	-2.332118	-2.743944	0.035957
1	-2.527702	-1.495745	-1.220048
1	-1.252769	-2.749007	-1.373296
6	-0.816560	2.521995	-0.733415
1	-1.022521	3.333624	-0.021406
1	0.035323	2.825143	-1.349373
1	-1.694342	2.411096	-1.383402
7	-0.854613	-1.268719	0.056870
7	-0.472584	1.301465	-0.029725
14	1.554258	0.311655	0.148432
1	0.126780	-0.833211	-1.688853
1	1.384861	0.600674	1.590200
6	3.046635	-0.875392	0.079486
1	3.271964	-1.188867	-0.946489
1	3.949091	-0.398987	0.479756
1	2.863954	-1.779765	0.670968

Reaction complex T2a

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.978910	-0.905344	-0.629328
6	-1.219785	1.137866	0.602710
6	0.081639	1.562059	0.376425
1	-1.945279	1.750599	1.114523
1	0.334230	2.565343	0.734160
6	-3.178003	-0.062985	-0.078937
1	-3.562766	0.015709	0.939615
1	-3.561085	0.766019	-0.676979
1	-3.478591	-1.015907	-0.510320
6	2.256278	1.478648	-0.572121
1	2.266728	2.544817	-0.316240
1	3.071164	0.980783	-0.031523
1	2.466884	1.371279	-1.642073
7	-1.707299	0.013782	-0.033455
7	0.985077	0.859449	-0.263023
14	0.897208	-1.225699	-0.417404
1	-1.577168	-1.642679	-1.163519
1	0.661203	-2.721916	-0.653849
6	1.538228	-1.309096	1.369593
1	1.878321	-2.313966	1.631009
1	2.347180	-0.597475	1.560769
1	0.718497	-1.042666	2.049260
1	1.878643	-1.019667	-1.525886

Reaction complex T2b

M062x/6-31G* optimized geometry (Å).

0 1			
6	1.022561	0.881290	-0.659832
6	1.015391	-1.164636	0.611713
6	-0.322222	-1.456293	0.489197
1	1.688343	-1.830090	1.129943
1	-0.643417	-2.412092	0.912194
6	3.089069	-0.309935	-0.259068
1	3.536506	-0.415086	0.731551
1	3.273792	-1.217232	-0.837640
1	3.515031	0.556408	-0.762368
6	-2.522552	-1.269975	-0.463126
1	-2.571136	-2.336368	-0.218843
1	-3.340510	-0.757850	0.059176
1	-2.685330	-1.150410	-1.541899
7	1.638207	-0.122197	-0.100505
7	-1.238618	-0.705797	-0.106342
14	-0.879146	1.147033	-0.457074
6	-0.720293	1.546552	1.436941
1	-0.143698	2.479417	1.476186
1	-1.680170	1.754248	1.929088
1	-0.205792	0.783836	2.033516
1	-1.005481	0.828266	-1.965382
1	1.668534	1.488782	-1.293882
1	-1.267469	2.603649	-0.739628

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.966509	-0.955518	-0.540847
6	-1.310897	1.162958	0.535575
6	-0.013533	1.610194	0.334351
1	-2.069986	1.782787	0.986260
1	0.197680	2.636768	0.650039
6	-3.200691	-0.189372	-0.033329
1	-3.586082	-0.023550	0.974217
1	-3.629646	0.548911	-0.713349
1	-3.449827	-1.197205	-0.359307
6	2.206465	1.548380	-0.496121
1	2.191922	2.613378	-0.236150
1	3.007978	1.058773	0.071451
1	2.455302	1.446454	-1.558611
7	-1.735527	-0.028458	-0.010173
7	0.936250	0.907429	-0.230949
14	0.936784	-1.172225	-0.441708
1	-1.536201	-1.768125	-0.990496
1	0.766515	-2.673282	-0.708846
6	1.729566	-1.348476	1.275563
1	0.972203	-1.737142	1.967159
1	2.532678	-2.091556	1.238290
1	2.119999	-0.418684	1.698151
1	1.841021	-0.888181	-1.598203

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

0 1			
6	-1.076653	-0.806997	-0.758496
6	-1.170243	1.207099	0.497250
6	0.135904	1.510488	0.298447
1	-1.639294	-1.536193	-1.337855
1	-1.809304	1.837478	1.098957
1	0.499679	2.423416	0.770455
6	-3.220808	-0.090401	0.173746
1	-3.375797	-0.437353	1.201148
1	-3.743736	0.858275	0.030293
1	-3.620778	-0.832781	-0.517733
6	2.409131	1.296722	-0.409772
1	2.429229	2.317597	-0.807280
1	2.865889	1.305228	0.591588
1	3.031545	0.674431	-1.059109
7	-1.798520	0.086682	-0.091596
7	1.051115	0.775832	-0.409303
14	0.744282	-1.039779	-0.378709
6	1.792346	-1.414436	1.165132
1	1.888026	-2.490574	1.330851
1	2.797842	-0.980075	1.106275
1	1.300556	-0.985058	2.046823
1	-0.371907	-2.194810	0.144863
1	1.341871	-1.655127	-1.588904

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.913859	-1.142591	-0.147904
6	-1.391876	1.236041	-0.143418
6	-0.124135	1.660642	-0.246464
1	-2.194630	1.937093	-0.343611
1	0.062093	2.691983	-0.532324
6	-3.195165	-0.344992	-0.022541
1	-3.822423	0.473824	0.340887
1	-3.393670	-0.490875	-1.098774
1	-3.486497	-1.256719	0.507112
6	2.278071	1.616439	0.083233
1	2.418640	2.261654	-0.793490
1	2.327606	2.245025	0.982786
1	3.117680	0.915477	0.113001
7	-1.800702	-0.055237	0.252814
7	1.027308	0.887972	-0.012580
14	0.851338	-0.785506	0.419423
6	2.110268	-1.852681	-0.473398
1	3.137226	-1.603050	-0.188406
1	1.955660	-2.910376	-0.234455
1	2.020051	-1.729066	-1.556967
1	-1.271798	-2.070188	0.315289
1	-0.934402	-1.300865	-1.243903
1	0.979662	-1.033123	1.882238

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NHC^{Me} + Me_2SiCl_2

Reaction complex C

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.757292	0.000025	-0.000108
6	-2.885377	-0.578825	-0.352914
6	-2.885743	0.577647	0.352565
1	-3.694652	-1.185055	-0.727175
1	-3.695384	1.183376	0.726848
6	-1.115225	2.104780	1.278198
1	-0.797399	1.829487	2.285580
1	-0.292093	2.559614	0.724129
1	-1.948287	2.805790	1.332800
6	-1.113849	-2.104685	-1.278742
1	-0.795014	-1.828648	-2.285613
1	-0.291247	-2.559837	-0.724145
1	-1.946784	-2.805740	-1.334700
7	-1.565850	0.919096	0.555677
7	-1.565293	-0.919529	-0.555908
14	1.176888	0.000276	-0.000007
6	2.069127	1.003645	1.315903
1	1.502119	1.010010	2.250517
1	3.006171	0.479496	1.531890
1	2.287440	2.023218	0.995539
6	2.070261	-1.003030	-1.315182
1	2.288702	-2.022472	-0.994501
1	1.504049	-1.009619	-2.250282
1	3.007321	-0.478576	-1.530331
17	0.971071	-1.782935	1.468925
17	0.971000	1.782981	-1.468757

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.627235	-0.479192	-0.135871
6	-1.997565	0.909395	1.113207
6	-1.312636	1.929784	0.502130
1	-2.806495	1.016617	1.820618
1	-1.677921	2.954115	0.594133
6	-2.981890	-1.145118	0.243479
1	-3.679874	-1.007362	1.070527
1	-3.451313	-0.805399	-0.684850
1	-2.722338	-2.200566	0.160185
6	-0.009463	2.495095	-1.417079
1	-0.643527	3.392956	-1.422342
1	1.043702	2.790348	-1.443974
1	-0.216733	1.938051	-2.339200
7	-1.788054	-0.353017	0.545070
7	-0.261107	1.642821	-0.267764
14	1.083578	-0.367418	0.637353
6	1.164768	0.630667	2.209391
1	0.283893	0.428506	2.827748
1	2.054754	0.337364	2.774848
1	1.199983	1.700060	2.000176
6	1.586072	-2.140226	1.012886
1	2.600262	-2.181135	1.422655
1	0.903464	-2.577230	1.751374
1	1.559307	-2.761601	0.112985
17	2.462803	0.264333	-0.786085
17	-0.710181	-1.447388	-1.606728

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	-1.095502	-0.208919	-0.066502
6	-1.184359	2.140689	0.066817
6	0.127526	2.308125	-0.212649
1	-1.827817	2.980558	0.275321
1	0.477514	3.338924	-0.271546
6	-3.296856	0.904744	-0.027397
1	-3.629871	1.924058	0.156402
1	-3.643259	0.573169	-1.007577
1	-3.693572	0.238020	0.737815
6	2.292746	1.799192	-1.076224
1	2.069671	2.618443	-1.764787
1	3.038527	2.134542	-0.346281
1	2.722566	0.982605	-1.659110
7	-1.822102	0.878986	0.010608
7	1.055240	1.343084	-0.438870
14	1.023624	-0.271307	0.398820
6	2.892359	-0.334464	0.833427
1	3.167759	0.512903	1.476734
1	3.064199	-1.249556	1.412186
1	3.581734	-0.361951	-0.014768
6	0.357277	-0.370116	2.181981
1	1.162953	-0.455934	2.916305
1	-0.220529	0.535797	2.409316
1	-0.317042	-1.224735	2.306213
17	-2.038087	-1.664983	-0.246543
17	1.127812	-1.966696	-0.895139

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.954800	-0.138298	-0.324660
6	0.624124	2.191356	-0.094363
6	-0.723991	2.148709	-0.153832
1	1.140230	3.116050	0.106634
1	-1.239792	3.097302	-0.019056
6	2.907654	1.298700	-0.142563
1	3.440480	0.801738	-0.952227
1	3.088272	2.370310	-0.191882
1	3.238219	0.902206	0.821370
6	-2.958029	1.290540	-0.405073
1	-3.381733	1.305409	0.606106
1	-3.184694	2.238335	-0.901859
1	-3.445419	0.492783	-0.971314
7	1.461551	1.065637	-0.269559
7	-1.514696	1.067068	-0.384742
14	-0.922222	-0.602303	-0.213071
6	-2.200434	-1.576779	0.769663
1	-2.524816	-1.029076	1.656092
1	-3.060552	-1.819086	0.132590
1	-1.756776	-2.515304	1.114495
6	-1.024176	-1.478715	-1.895326
1	-0.720188	-2.528714	-1.806899
1	-2.058193	-1.481252	-2.260335
1	-0.395121	-1.010991	-2.659793
17	0.220207	-0.482714	2.131056
17	2.054118	-1.449609	-0.580108

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1			
6	0.807769	-0.118859	0.074912
6	0.091410	2.027058	-0.749941
6	-1.221830	1.882131	-0.511808
1	0.447973	2.969944	-1.146033
1	-1.869907	2.737240	-0.696471
6	2.445159	1.653943	-0.370549
1	2.615446	2.420653	-1.129209
1	2.518971	2.104779	0.626905
1	3.209248	0.884513	-0.476623
6	-2.989082	0.854131	0.795465
1	-2.673285	1.204124	1.786685
1	-3.708165	1.574775	0.386694
1	-3.503045	-0.103213	0.912292
7	1.124880	1.067528	-0.593617
7	-1.864091	0.703567	-0.112581
14	-0.952553	-0.747862	-0.383431
6	-1.484207	-2.139595	0.733705
1	-2.439445	-2.564634	0.408796
1	-0.735490	-2.938030	0.705736
1	-1.579780	-1.801836	1.768808
6	-0.900214	-1.202131	-2.193801
1	-0.192378	-2.013769	-2.384839
1	-1.890544	-1.516009	-2.538552
1	-0.593878	-0.332997	-2.784366
17	0.829978	0.106498	1.942006
17	2.017697	-1.417863	-0.282964

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NHC^{Me} + $SiCl_4$

Reaction complex C

M062x/6-31G* optimized geometry (Å).

0 1			
6	1.043571	-0.000150	-0.000088
6	3.166101	-0.669899	-0.106303
6	3.166481	0.668324	0.105907
1	3.974499	-1.373762	-0.222235
1	3.975283	1.371764	0.221617
6	1.393608	2.437900	0.373487
1	0.701293	2.711113	-0.424950
1	0.898227	2.520791	1.342315
1	2.267980	3.087580	0.346821
6	1.392129	-2.438413	-0.373661
1	0.700911	-2.711815	0.425665
1	0.895317	-2.520583	-1.341818
1	2.266309	-3.088432	-0.348743
7	1.846943	1.063243	0.163613
7	1.846301	-1.064014	-0.163858
14	-0.893530	0.000169	-0.000083
17	-1.948651	-1.624700	-0.756769
17	-0.699247	-0.927780	2.005858
17	-1.946643	1.625959	0.757309
17	-0.699249	0.927686	-2.005920

Reaction complex T2

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.942083	-0.422794	-0.093170
6	-1.846555	1.551422	-0.806714
6	-1.110701	2.030588	0.210109
1	-2.430898	2.129914	-1.508700
1	-1.075056	3.076292	0.494517
6	-3.246715	-0.438780	-1.034092
1	-3.756219	0.125070	-1.817161
1	-3.154125	-1.477075	-1.351532
1	-3.829326	-0.383061	-0.108340
6	-0.377257	1.251087	2.392223
1	-1.235789	1.851879	2.705605
1	-0.454903	0.263701	2.855951
1	0.554628	1.714614	2.729288
7	-1.915798	0.149000	-0.873341
7	-0.371405	1.092005	0.936263
14	0.885918	-0.012945	-0.163735
17	1.952771	-0.623761	1.497266
17	1.701670	1.636380	-1.117032
17	1.515095	-1.497995	-1.546729
17	-1.397235	-1.846170	0.804263

Reaction complex E

M062x/6-31G* optimized geometry (Å).

0 1			
6	1.276064	-0.183978	-0.175028
6	1.438417	2.144067	0.167209
6	0.150891	2.381839	-0.157602
1	2.095830	2.928223	0.506361
1	-0.184271	3.416970	-0.122765
6	3.498052	0.818708	0.076634
1	3.868649	1.819231	0.286997
1	3.804802	0.129790	0.864183
1	3.887580	0.473655	-0.881746
6	-1.971877	2.027710	-1.191532
1	-1.656521	2.803880	-1.893250
1	-2.487858	1.246550	-1.748860
1	-2.666885	2.442979	-0.456182
7	2.024541	0.870802	0.021145
7	-0.776875	1.463441	-0.545745
14	-0.738850	-0.212404	0.072751
17	-0.933500	-1.672186	-1.410574
17	-2.841816	-0.241400	0.574965
17	-0.210238	-0.652212	2.088629
17	2.138474	-1.655226	-0.442380

Reaction complex T3

M062x/6-31G* optimized geometry (Å).

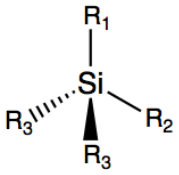
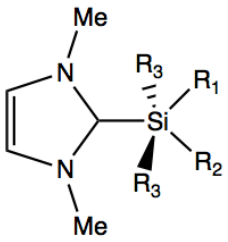
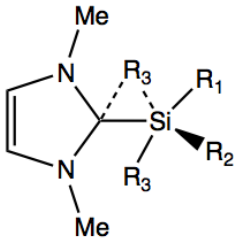
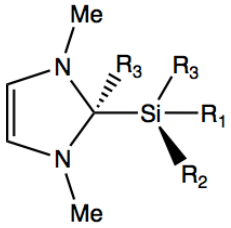
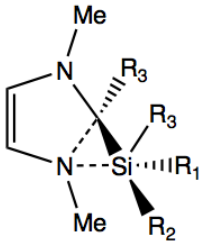
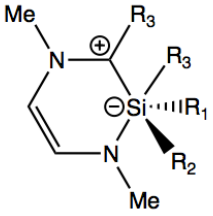
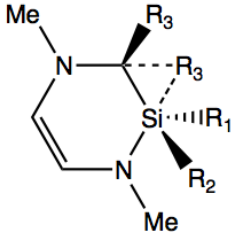
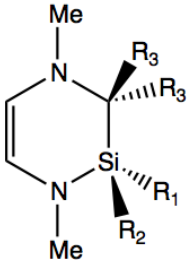
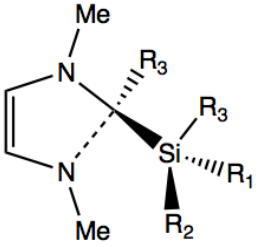
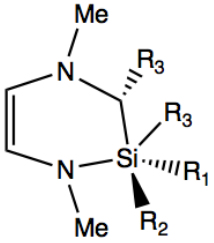
0 1			
6	-1.076764	-0.333337	-0.096654
6	-1.255085	1.966213	-0.671667
6	0.044958	2.296920	-0.535095
1	-1.969831	2.720442	-0.962370
1	0.292305	3.345305	-0.687232
6	-3.285644	0.654389	-0.265355
1	-3.496739	0.680442	0.808361
1	-3.713118	1.528314	-0.753128
1	-3.703020	-0.248116	-0.708171
6	2.304114	2.075188	0.342055
1	2.451067	3.078431	-0.067969
1	2.193666	2.137323	1.430099
1	3.183478	1.474843	0.101560
7	-1.829244	0.683617	-0.455908
7	1.116783	1.479608	-0.268532
14	0.791101	-0.217060	-0.189140
17	2.170623	-1.350356	0.791260
17	1.031494	-0.913478	-2.157017
17	-0.322910	0.208235	2.164703
17	-1.803646	-1.872459	0.137416

Reaction complex F

M062x/6-31G* optimized geometry (Å).

0 1			
6	-0.993305	-0.203015	-0.110452
6	-0.936827	2.102995	0.563695
6	0.335610	2.357562	0.232345
1	-1.573795	2.930386	0.845645
1	0.679302	3.386262	0.253545
6	-3.036161	0.906403	0.671617
1	-3.319285	1.686417	1.379806
1	-3.453578	1.137359	-0.316471
1	-3.439422	-0.041502	1.024809
6	2.626507	1.913927	-0.494002
1	2.532504	2.621757	-1.323510
1	3.115400	2.411875	0.350748
1	3.257999	1.086691	-0.824039
7	-1.574674	0.838820	0.630501
7	1.311957	1.408152	-0.118194
14	0.897544	-0.220215	0.140141
17	-1.661679	-1.802845	0.341377
17	1.292036	-0.875246	2.045703
17	1.864639	-1.462011	-1.152208
17	-1.289153	0.002909	-1.947688

Orientations of optimised structures (B1-B7)

B		**C**	
T1		**D**	
T2		**E**	
T3		**F**	
T2a		**T2b**	

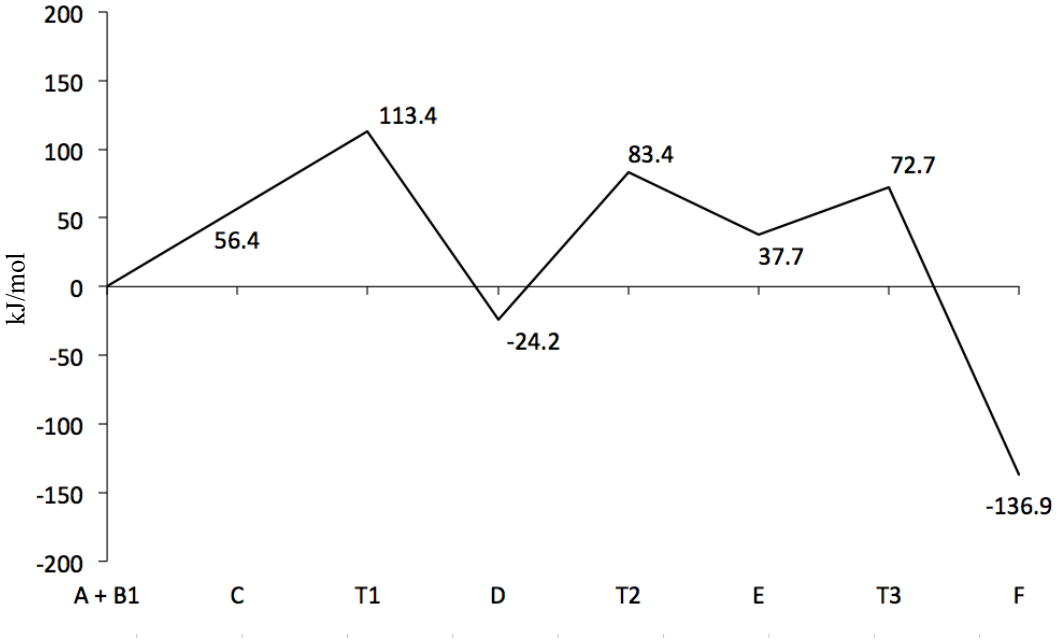
B1: R_1/R_2 = Ph, R_3 = H
B2: R_1 = Ph, R_2/R_3 = H
B3: R_1/R_2 = Ph, R_3 = Cl
B4: R_1/R_2 = Me, R_3 = H
B5: R_1 = Ph, R_2/R_3 = H
B6: R_1/R_2 = Ph, R_3 = Cl
B7: $R_1/R_2/R_3$ = Cl

* Please note structure **C** is not applicable for **B4** and **B5**; structures **T1** and **D** are not applicable for **B3**, **B6** and **B7;** structures **T2a** and **T2b** are not applicable for **B1**, **B2**, **B3**, **B6** and **B7**.

Free energy profiles

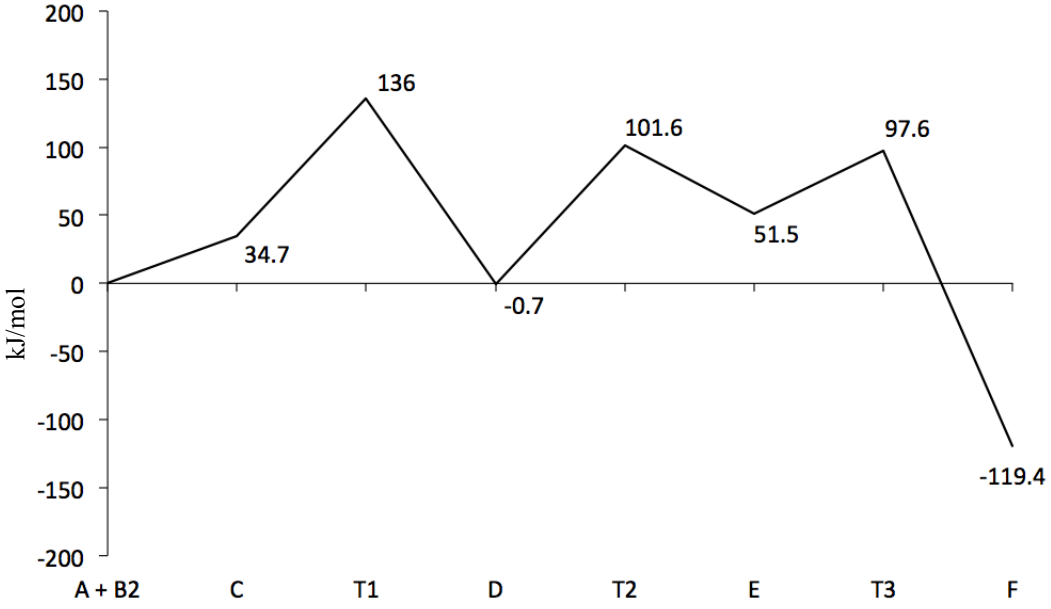
B1

NHC^{Me} + Ph_2SiH_2 Reaction Pathway



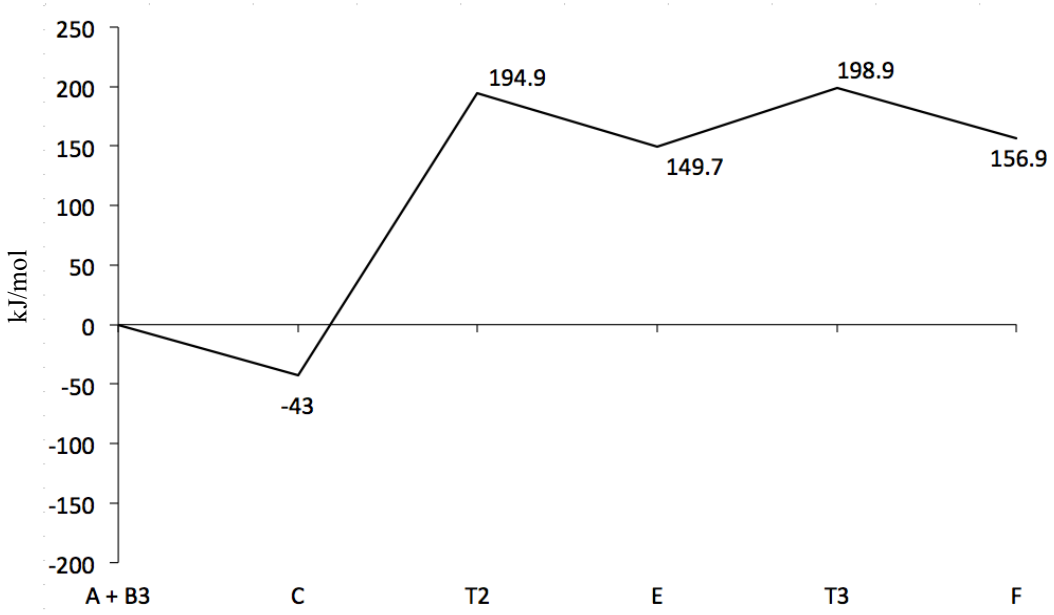
B2

NHC^{Me} + $PhSiH_3$ Reaction Pathway



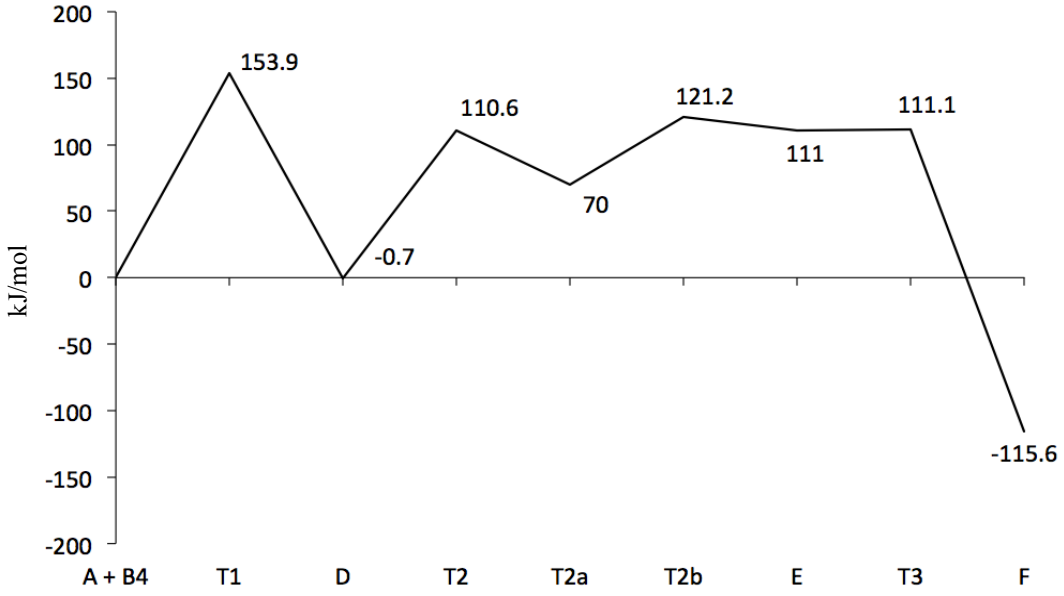
B3

NHC^{Me} + Ph_2SiCl_2 Reaction Pathway



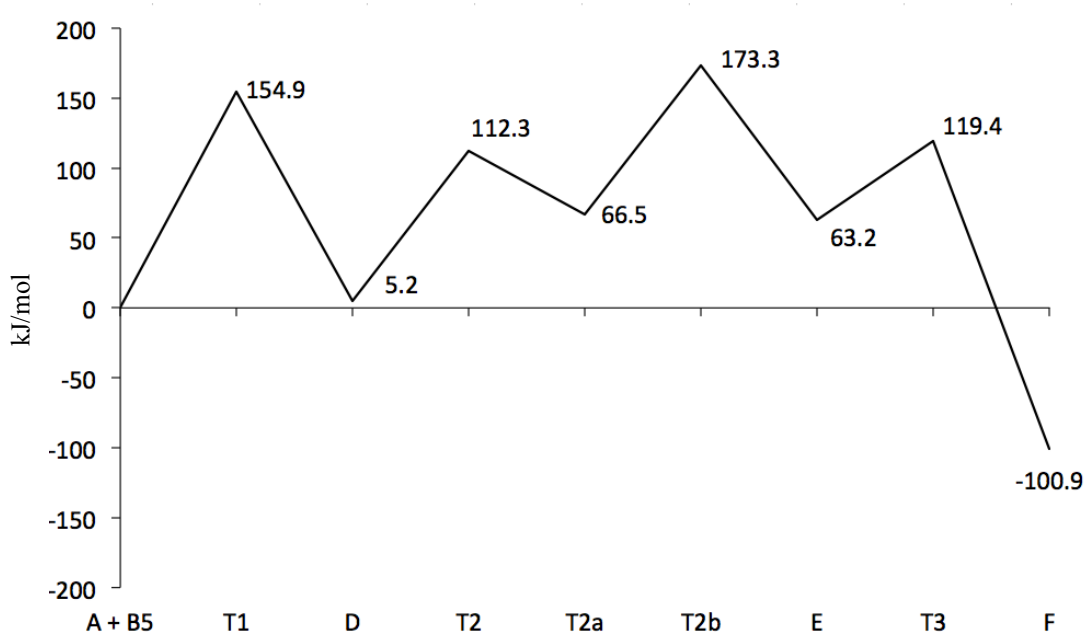
B4

NHC^{Me} + Me_2SiH_2 Reaction Pathway



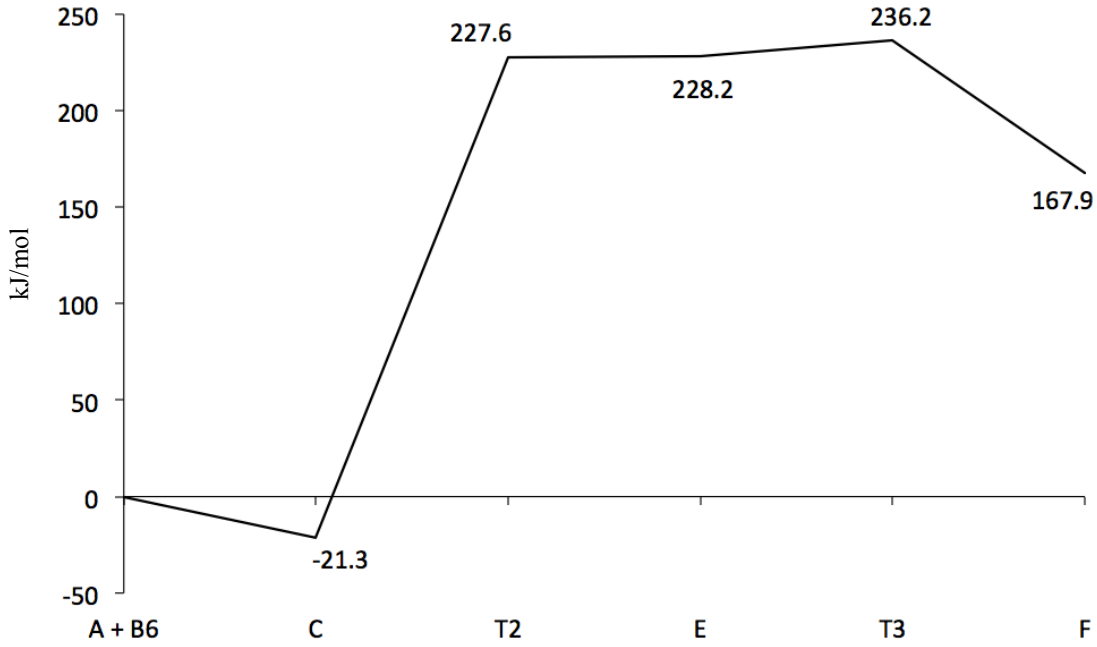
B5

NHC^{Me} + $MeSiH_3$ Reaction Pathway



B6

NHC^{Me} + Me_2SiCl_2 Reaction Pathway



B7

NHC^{Me} + $SiCl_4$ Reaction Pathway